Discrete element modelling and experimental validation of a granular solid subject to different loading conditions

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Declaration

This thesis is submitted to The University of Edinburgh for the degree of Doctor of Philosophy. The research work described and reported in this thesis has been completed solely by Yun-Chi Chung under the supervision of Professor Jin Y. Ooi. Where other sources are quoted full references are given.

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Abstract

Many of the materials handled by industry each year are of a granular or particulate nature. These include pharmaceutical powders, chemical pellets, agricultural grains, coals and other minerals, sands and gravels. In recent years, the Discrete Element Method (DEM) has been used extensively to investigate the behaviour of granular solids subjected to a variety of loading conditions. However, the majority of the numerical computations were often not validated or compared with experimental results and there is a question as to whether DEM is capable of producing quantitative predictions rather than only qualitative representation of a particulate assembly. It is thus useful to verify DEM calculations and to investigate the relative importance of the DEM input parameters for producing satisfactory predictions. The aim of this study was to simulate spherical (glass beads) and non-spherical (corn grains) particles under a variety of loading scenarios and to validate against physical experiments. Secondary objective was to explore the influence of the particle scale (micro) parameters on the bulk scale (macro) responses.

The study commenced with the development of physical calibration experiments for the DEM validation. These were filling of a model silo, confined compression in a cylinder, rod penetration into a granular bulk and silo discharging through an outlet. These actions on a granular system can be expected to occur in a wide range of industrial processes and are relevant for the industrial sponsor Deere & Co. Key observations were made in each of the tests and compared with the corresponding DEM simulations.

To achieve a high level quantitative validation, the grains properties required for DEM simulations were not simply assumed but measured directly. The
methodologies and apparatuses for measuring the main particle parameters (Young's modulus, friction coefficient and restitution coefficient) for DEM models were devised. Measurements of the mechanical and geometric properties were made for the glass beads and the corn grains for the DEM simulations. In addition, measurements were also made on many samples of corn and wheat, providing a database of measurements that can be used for future simulations of grain dynamics.

The DEM simulations were conducted using two commercial software: PFC3D and EDEM, the latter being the DEM software that originated from Edinburgh University. A set of 8 benchmark tests were carried out to validate the codes and to evaluate the fundamental aspects of DEM. Following that, a large number of DEM simulations were conducted and comparisons between DEM simulations and experiments were made. For corn grains: the study shows that 4-sphere representation together with the measured corn properties produced satisfactory match with experiments for silo filling (normal wall pressure distribution), confined compression (normal wall pressure distribution, load transfer to boundary surfaces, and silo design parameters $K$ and $\mu_{\text{bulk}}$), rod penetration (force-displacement response) and silo discharge (mass flow rate and angle of repose). For glass beads: the DEM simulations also gave good agreement with experiments for silo filling (normal wall pressure distribution), confined compression (normal wall pressure distribution, load transfer to boundary surfaces), rod penetration (force-displacement response) and silo discharge (mass flow rate). These findings provide sound verification that DEM is capable of producing quantitative predictions of the problems studied. They also suggest that very accurate representation of the non-spherical particle shape may not be necessary to produce satisfactory predictions and capturing the linear dimensions of a particle may be adequate.

Two DEM results that produced larger discrepancies with experiments are filling density (~17% lower for corn grains and ~8% lower for glass beads) and loading stiffness (stiffer response). Plausible explanations for these are given in this thesis, which should be explored further.
The influence of DEM input parameters was explored extensively to study the sensitivity of single particle (micro) properties on the bulk (macro) behaviour of a dense granular system. This study has resulted in many useful observations with significant implications for the relative importance of the DEM input parameters. The chief conclusions include

1. Sensitivity to initial packing structure varies depending on the parameter of interest. For corn grains, DEM results were found to be not so sensitive to the particle spacing used in particle generation.
2. Whilst particle stiffness directly influences the bulk stiffness of the system during confined compression, it has a much smaller influence on the boundary contact forces. Reducing stiffness up to $10^4$ times produced no effect on the average rod penetration force, whilst providing a huge computational advantage.
3. The non-linear influence of inter-particle friction on bulk friction has been established, providing a basis for explaining several phenomena observed.
4. Rod penetration force does not depend significantly on rod friction for up to 60 mm penetration. The resistance of a rod penetrating into a granular body appears to come from the mobilisation of internal friction in the granular assembly adjacent to the rod and not from the surface friction of the rod.
5. A power law relationship between particle stiffness and bulk stiffness has been derived from the DEM results for confined compression of glass beads.

The influence of gravity on the bulk response of a dense granular medium has been examined for several load cases. The magnitude of the gravitational acceleration $g$ was found to have no noticeable effect on the force transmission in the confined compression. The gradient of the force-displacement response in rod penetration was proportional to $g$ and the mass flow rate in silo discharge was proportional to the square root of $g$. These are in agreement with the expectations.

One method to evaluate the effect of the particle forces acting on the contacting body is to link the DEM simulation outcomes to a finite element package. A methodology to link the DEM simulation results with the finite element method was developed. A verification example showed that this Fortran program was coded correctly.
simple example was used to demonstrate how this can be used to determine the stresses in the contacting body resulting from the particle forces.
Publications

Parts of this research have been presented in the following publications, which are given in Appendix G.


The following technical reports have been produced for the industrial sponsor Deere & Company.


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### Nomenclature

**Roman characters**

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<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a, b)</td>
<td>Major and minor radii in the contact ellipse of the two contacting bodies</td>
</tr>
<tr>
<td>(A, B)</td>
<td>Constants depending on the magnitudes of the principal curvatures of the surface in contact and on the angle between the planes of principal curvatures of the two surfaces.</td>
</tr>
<tr>
<td>([A]_{\text{I}})</td>
<td>Nodal displacements in a triangular plate element</td>
</tr>
<tr>
<td>(C, k)</td>
<td>Beverloo constants</td>
</tr>
<tr>
<td>(d)</td>
<td>Diameter of the particle</td>
</tr>
<tr>
<td>(D)</td>
<td>Diameter of the cylinder</td>
</tr>
<tr>
<td>(D_o)</td>
<td>Diameter of the orifice</td>
</tr>
<tr>
<td>(e)</td>
<td>Coefficient of restitution</td>
</tr>
<tr>
<td>(e_E)</td>
<td>Energy restitution coefficient</td>
</tr>
<tr>
<td>(e_n)</td>
<td>Normal coefficient of restitution</td>
</tr>
<tr>
<td>(e_r)</td>
<td>Resultant restitution coefficient</td>
</tr>
<tr>
<td>(e_t)</td>
<td>Tangential coefficients of restitution on the centre of mass</td>
</tr>
<tr>
<td>(E)</td>
<td>Young's modulus of the grain</td>
</tr>
<tr>
<td>(E_{\text{bulk}})</td>
<td>Bulk Young's modulus of the granular solid respectively</td>
</tr>
<tr>
<td>(E_{\text{in}})</td>
<td>Kinetic energies before impact</td>
</tr>
<tr>
<td>(E_{\text{out}})</td>
<td>Kinetic energies after impact</td>
</tr>
<tr>
<td>(E_w)</td>
<td>Young's modulus of the cylinder</td>
</tr>
</tbody>
</table>
$f_n$ Normal contact force
$f_t$ Tangential contact force
$F_b$ Measured force at the bottom platen
$F_{CN}$ Normal component of the contact force
$F_{CN,S}$ Normal spring force
$F_{CN,D}$ Normal damping force
$F_{CT}$ Tangential component of the contact force
$F_{CT,S}$ Tangential spring force
$F_{CT,S,(n-1)}$ Spring force at the previous time step
$F_{CT,D}$ Tangential damping force
$F_n$ Normal linear impulse
$F_T$ Applied load at the top platen
$F_t$ Tangential linear impulse
$F_x, F_y$ In-plane forces in a plate
$F_z$ Normal force in a plate
$\bar{F}$ Resultant force vector, the sum of all contact forces
$\{F_{con, nodal}\}_{1x1}$ Equivalent nodal forces in the global coordinate system
$\{F_{con, P}\}_{6x1}$ Resultant contact forces in the global coordinate system
$g$ Gravity constant
$\bar{g}$ Gravity acceleration vector
$G$ Shear modulus of the particle
$G_c$ Mass centre of the particle
$h$ Height of the granular solid
$H$ Angle between the normal planes containing the curvatures $1/R_1$ and $1/R_2$
$H_r$  Bounce height at position B
$	ilde{H}$  Angular momentum
$\dot{H}$  Time rate of change of the angular momentum
$I_{ij}$  Moments and products of inertial
$k_n$  Normal contact stiffness
$k_t$  Tangential contact stiffness
$\kappa$  Lateral pressure ratio
$K_c$  Geometric constant
$K_{contact}$  Contact spring stiffness
$K_n$  Hertz contact constant
$m$  Total mass of the particle
$m^*$  Equivalent mass
$m_i$  Mass of sphere $i$
$m_j$  Mass of sphere $j$
$M_{x}, M_{y}$  Bending moments in plate
$M_z$  Concentrated torque in plate
$\bar{M}_G$  Resultant moment vector taken about the mass centre
$\bar{n}$  Unit normal vector joining the centre of Sphere 2 to the centre of Sphere 1 at contact
$[N]_{load}$  Shape function matrix for a 3-node plate element
$q_T$  Mean vertical pressure applied at the top boundary ($z=0$)
$r^*$  Equivalent radius
$r_i$  Radius of sphere $i$
$r_j$  Radius of sphere $j$
$r_i$  Radius of sphere 1
$r_2$  Radius of sphere 2

$r_{\text{min}}$  Radius of the minimum size particle in the assembly

$R_1, R'_1$  Principal radii of curvature at the point of contact for Body 1

$R_2, R'_2$  Principal radii of curvature at the point of contact for Body 2

$t$  Thickness of the cylinder

$t_{\text{duration}}$  Contact duration

$\vec{t}$  Unit vector for the tangential direction

$[T]$  $3 \times 3$ transformation matrix

$[T_{\text{trans,2}}]$  $6 \times 6$ transformation matrix

$[T_{\text{trans,3}}]$  $18 \times 18$ transformation matrix

$u_x, u_y, u_z$  Displacements in the x, y and z directions

$V_{cn}$  Relative normal velocities immediately before impact

$V'_{cn}$  Relative normal velocities immediately after impact

$V_{cn,1}$  Pre-collision normal velocity at its centre of mass for Sphere 1

$V_{cn,2}$  Pre-collision normal velocity at its centre of mass for Sphere 2

$V'_{cn,1}$  Post-collision normal velocity for Sphere 1

$V'_{cn,2}$  Post-collision normal velocity for Sphere 2

$V_{ct}$  Relative tangential velocities at the centre of mass immediately before impact

$V'_{ct}$  Relative tangential velocities at the centre of mass immediately after impact

$V'_{ct,1}$  Post-collision tangential velocity for Sphere 1

$V'_{ct,2}$  Post-collision tangential velocity for Sphere 2

$V_{in}$  Incoming velocity

$V_{in,N}$  Normal component of the incoming velocity
$V_{in,T}$ Tangential component of the incoming velocity

$V_{out}$ Rebounding velocity

$V_{out,N}$ Normal component of the rebounding velocity

$V_{out,T}$ Tangential component of the rebounding velocity

$V_{out,X}$ Linear velocity in the x direction after rebound

$V_{out,Y}$ Linear velocity in the y direction after rebound

$V_{out,Z}$ Linear velocity in the z direction after rebound

$V_{st}$ Relative tangential velocities at the contact point immediately before impact

$V'_{st}$ Relative tangential velocities at the contact point immediately after impact

$V_{st,1}$ Pre-collision tangential velocity at its centre of mass for Sphere 1

$V_{st,2}$ Pre-collision tangential velocity at its centre of mass for Sphere 2

$V'_{st,1}$ Post-collision tangential velocity on contact path for Sphere 1

$V'_{st,2}$ Post-collision tangential velocity on contact path for Sphere 2

$V_{relative,n}$ Normal relative velocity

$V_{relative,t}$ Tangential relative velocity

$\{U\}_{6x1}$ Displacement field in a triangular plate element

$W$ Mass flow rate

$x_G$ Position vector of the mass centre

$\dot{x}_G$ Velocity vector of the mass centre

$\ddot{x}_G$ Acceleration vector of the mass centre

$z$ Distance below the equivalent surface at full storage condition
\( z_o \) Janssen reference depth

**Greek characters**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \alpha_n )</td>
<td>Normal contact displacement (overlap)</td>
</tr>
<tr>
<td>( \beta_d )</td>
<td>A damping ratio</td>
</tr>
<tr>
<td>( \beta )</td>
<td>Tangential coefficients of restitution based on the contact point</td>
</tr>
<tr>
<td>( \gamma )</td>
<td>Bulk density of a granular solid</td>
</tr>
<tr>
<td>( \Delta F_{CT,S} )</td>
<td>Increment of the tangential spring force</td>
</tr>
<tr>
<td>( \Delta \alpha_t )</td>
<td>Incremental tangential displacement</td>
</tr>
<tr>
<td>( \Delta t )</td>
<td>Time step</td>
</tr>
<tr>
<td>( \Delta t_c )</td>
<td>Critical time step</td>
</tr>
<tr>
<td>( \varepsilon_a )</td>
<td>Axial strain of the cylinder at the measuring points</td>
</tr>
<tr>
<td>( \varepsilon_r )</td>
<td>Radial strain of the granular solid</td>
</tr>
<tr>
<td>( \overline{\varepsilon_v} )</td>
<td>Mean vertical strain</td>
</tr>
<tr>
<td>( \varepsilon_z )</td>
<td>Vertical strain of the granular solid</td>
</tr>
<tr>
<td>( \varepsilon_\theta )</td>
<td>Average hoop strain of the cylinder at the measuring points</td>
</tr>
<tr>
<td>( \theta )</td>
<td>Angle of the inclination of the base plate</td>
</tr>
<tr>
<td>( \theta_x, \theta_y, \theta_z )</td>
<td>Rotations in the x, y and z directions</td>
</tr>
<tr>
<td>( \vec{\lambda} )</td>
<td>Unit normal vector of the plane where the normal and tangential contact forces occur</td>
</tr>
<tr>
<td>( \mu )</td>
<td>Coefficient of friction</td>
</tr>
<tr>
<td>( \mu_{bulk} )</td>
<td>Bulk wall friction coefficient</td>
</tr>
<tr>
<td>( \nu )</td>
<td>Poisson’s ratio of the particle</td>
</tr>
<tr>
<td>( \nu_{bulk} )</td>
<td>Bulk Poisson’s ratio of the granular solid</td>
</tr>
<tr>
<td>( \nu_w )</td>
<td>Poisson’s ratio of the cylinder</td>
</tr>
</tbody>
</table>
\( \rho \)  
Density of the particle

\( \rho_b \)  
Bulk density of the solid

\( \omega_1 \)  
Pre-collision angular velocity for sphere 1

\( \omega_2 \)  
Pre-collision angular velocity for sphere 2

\( \omega'_1 \)  
Post-collision angular velocity for sphere 1

\( \omega'_2 \)  
Post-collision angular velocity for sphere 2

\( \omega_x \)  
Angular velocity in the x direction

\( \omega_y \)  
Angular velocity in the y direction

\( \omega_z \)  
Angular velocity in the z direction

\( \bar{\omega} \)  
Angular velocity vector of the particle

\( \bar{\omega}_0 \)  
Initial angular velocity

\( \dot{\omega} \)  
Angular acceleration vector of the mass centre

\( \chi \)  
A function of the Poisson's ratio

\( \bar{\sigma}_v \)  
Average vertical stress in the bulk solid

\( \sigma_h \)  
Mean horizontal stress in the bulk solid

\( \sigma_\theta \)  
Hoop stress of the granular solid

\( \bar{\tau} \)  
Average shear stress in the bulk solid

\( \partial W \)  
External virtual work
Chapter 1

Introduction

1.1 General background

There are many processes in the agricultural industry in which the grains undergo a variety of stress and deformation regimes. These include seeding, harvesting, conveying, transporting and storing, to name a few. A better modelling and understanding of the behaviour of agricultural grains should lead to improved methods for these handling processes. It is proposed that the Discrete Element Method (DEM) computer simulations be used to model such processes. DEM is by now a well-established method for modelling granular assemblies and is being used extensively in both scientific and industrial applications (e.g. silo flow: Hirshfeld and Rapaport, 2001; Sanad et al., 2001; Yang and Hsiau, 2001; Cleary and Sawley, 2002; Li et al., 2004; ball mill operation: Venugopal and Rajamani, 2001; Mio et al., 2002; Monama and Moys, 2002; Cleary et al., 2003; Mishra, 2003a and 2003b; fluidised beds: Hoomans et al., 2001; Potapov et al., 2001; Kafui et al., 2002; Kuwagi and Horio, 2002; Lyczkowski and Bouillard, 2002). Although DEM has been shown to be a very promising tool, careful validations of the simulation outcomes are rather rare and there is a question as to whether DEM is capable of producing quantitative predictions rather than only qualitative representation of the particulate assembly. In addition, the input parameters used in the DEM simulations were often simply given without any explanation as to where they came from, and seldom measured in
laboratory tests, so influence of the input parameters on the prediction outcomes can be rather obscure. Therefore, validations against experimental observations are needed to establish the validity of DEM results. This thesis presents a validation study of DEM with closely matching sets of numerical and physical experiments, conducted with careful measurements of the input parameters.

1.2 Objectives and scope of this research

The aim of this research was to simulate spherical (glass beads) and non-spherical (corn grains) grains under a variety of loading scenarios and to validate against physical experiments. Secondary objective was to explore the influence of the particle (micro) scale parameters on the bulk (macro) scale responses. The additional brief study of the gravity effect on the bulk behaviour was motivated by the increased research relating to lunar and Martian exploration. An attempt was also made to develop the methodology for linking the DEM simulation outcomes to the finite element method for determining the stresses in the contacting body. As the project was funded by a company, the loading scenarios studied were chosen to reflect the types of loading actions that prevail in the handling processes in agricultural industry. These loading cases were also designed to be sufficiently well defined for more in-depth scientific examination of the basic phenomena.

The key tasks for this research are:

1. Develop and conduct physical calibration experiments of silo/cylinder filling, confined compression, rod penetration and silo discharge;
2. Develop methods to measure particle parameters for DEM models and conduct measurements for samples of corn, wheat and glass beads;
3. Conduct a large number of DEM simulations and compare with experiments;
4. Study the influence of DEM input parameters;
5. Examine the influence of the gravity on the bulk responses of a granular assembly;
6. Develop the methodology to link DEM with FEA.
1.3 Structure of the thesis

The thesis is divided into ten Chapters. A brief introduction for each chapter is described below.

Chapter 1 presents the background, objectives and scope of this research. The layout of the thesis is summarised.

Chapter 2 reviews the literature regarding this study. The literature review focuses on benchmark tests for validating DEM codes, input parameters for DEM simulations, contact force models, representation for non-spherical particles, experimental validation of the DEM and linking DEM with FEA.

Chapter 3 gives a brief review of the DEM methodology. Several issues that are important for this present study and for achieving satisfactory predictions are discussed. These include the Hertz-Mindlin with no slip contact model, the multiple sphere method for representing non-spherical particles and the determination of the computational time step.

Chapter 4 describes the careful benchmark testing of the DEM codes used in this thesis, namely EDEM (DEM Solutions, 2005) and PFC3D (Itasca, 2003). It reviews the analytical solutions for elastic normal and oblique impacts. A set of eight benchmark tests were performed and the DEM results in these benchmark tests are compared with the analytical solutions, experimental results or finite element analysis results found in the literature.

Chapter 5 presents the methodologies and experimental apparatuses to measure the main particle parameters (Young’s modulus, friction coefficient and coefficient of restitution) for DEM models. Measurements of the physical and mechanical properties for samples of corn, wheat and glass beads are also reported in this chapter.
Chapter 6 describes physical experiments of silo filling, confined compression, rod penetration and silo discharging. The corresponding DEM simulations are conducted and comparison between numerical results and experimental results is made.

Chapter 7 explores the influence of DEM input parameters to study the sensitivity of single particle (microscopic) properties on the bulk (macroscopic) behaviour of a dense granular system. The DEM input parameters studied include the particle generation scheme (initial packing structure), particle elastic stiffness, inter-particle friction and particle-boundary friction. A simple approach is proposed to determine the relationship between particle stiffness and bulk stiffness in a dense particle assembly.

Chapter 8 examines the influence of gravity on the bulk responses of a granular solid.

Chapter 9 describes a methodology to link the DEM simulation results with the finite element method in order to evaluate the effect of the particle forces acting on the contacting body. A verification example is given to ensure that the Fortran program is coded correctly.

In Chapter 10, general conclusions are drawn from this study and recommendations for further research and potential applications are discussed.
Chapter 2

Literature review

2.1 Introduction

Discrete element method (DEM) is an increasingly popular numerical technique for simulating the mechanical behaviour of discrete particle assemblies (Cundall and Strack, 1979). It is usually based on the use of an explicit numerical scheme in which the interactions between a finite number of particles are monitored contact by contact and the motion of the particles is modelled particle by particle. The particles deform locally at the contact points by means of an overlap, commonly known as the soft contact method. By comparison with static continuum analysis, Newton's equations of motion for each particle effectively replace the equilibrium equations used in continuum mechanics, and the model of inter-particle contacts replaces the constitutive model. The essential feature of this approach is that each particle is modelled separately, so the integrated behaviour of the mass should be accurately represented, without the need for control tests to establish constitutive models for the bulk behaviour. The discrete element scheme is based on the idea that a small enough time step should be chosen to ensure that, during a single time step, disturbances do not propagate from any particle further than its immediate neighbours. DEM has the capacity of modelling the material at the microscopic level and analysing multiple interacting bodies undergoing large displacements and
rotations, thus capturing all the phenomena that pertain to the particulate nature of granular mediums.

Following the pioneering work of Cundal and Strack (1979), many researchers have used, examined and improved the discrete element method for the past twenty years. The fields of study can be mainly categorized as follows:

1. Fundamental investigation and application of the DEM in granular soils, rocks, pharmaceutical powders, chemical pellets, agricultural grains, coals and other minerals;
2. Development of improved contact force models;
3. Development of representation for non-spherical particles and complex boundary geometry;
4. Experimental validation of the DEM;
5. Development of coupled modelling methods for example, DEM & Finite Element Method (FEM) and DEM & Computational Fluid Dynamics (CFD);
6. Large-scale industrial applications of DEM.

A concise review of the relevant literature for this thesis is presented below on the following aspects: (1) benchmark tests for validating DEM codes; (2) input parameters for DEM simulations; (3) contact force models; (4) representation for non-spherical particles; (5) experimental validation of the DEM; and (6) linking DEM and FEA. These aspects are described below.

### 2.2 Benchmark tests for validating DEM codes

Discrete element method was proposed by Cundal and Strack in 1979, but until the past ten years, the literature on DEM validation focuses on elementary case of collision of a sphere with a flat wall to verify different contact models and to validate DEM codes.

Vu-Quoc and Zhang (1999a) proposed an improved tangential force-displacement model for an elastic frictional contact in 3D discrete element simulation of a dry
particulate system. To validate their DEM code, simulations were carried out for a benchmark test of 100 hard spherical particles colliding with a rigid planar surface. These 100 hard spheres were given the same initial translational velocity perpendicular to the rigid surface and subjected to different angular velocities so that the spheres have different incident angles. The numerical results were compared with solutions by dynamic principles. Kharaz et al. (2001) conducted a drop test for aluminium oxide spheres impacting a thick soda-lime glass anvil over impact angles from normal to very near glancing incidence and calculated the normal and tangential restitution coefficients. The experimental results were compared with the simple theoretical model and numerical results of Maw et al. (1976). Zhang and Vu-Quoc (2002) modelled the dynamic process of normal collision between a deformable sphere and a frictionless rigid planar surface using finite element analysis. Both elastic material and elasto-perfectly plastic material were considered. The results from the elastic material were compared to Hertz contact theory (1896), whilst the results for elasto-plastic collisions in FEA model were compared with the results of DEM simulations using Vu-Quoc and Zhang (1999b) elasto-plastic normal force-displacement model. Wu et al. (2003) performed a finite element analysis of both elastic and elasto-plastic oblique impacts of a sphere with a target wall. For elastic oblique impacts, the results are in complete agreement with previous study. However, for elasto-plastic oblique impacts, the normal coefficient of restitution is not only a function of the normal impact velocity, but also depends on the impact angle. The FEA results were compared with dynamic principles, Hertz theory and numerical results from Maw et al. (1976). Renzo and Maio (2004) investigated the influence of different contact models on the accuracy of the simulated collision process. In their work, three contact force models: i) a linear model based on a Hooke-type relation; ii) a non-linear model based on the Hertz theory for the normal direction and the no-slip solution of the theory developed by Mindlin and Deresiewicz (1953) for the tangential direction; iii) a non-linear model, based on the complete theory of Hertz and Mindlin & Deresiewicz, are applied to the basic case of an elastic-frictional collision of a sphere with a flat wall. The results were compared with the data provided by the experiments of Kharaz et al. (2001) and with the approximated analytical solution derived by Maw et al. (1976).
Table 2.1 shows a summary of the literature review for these benchmark tests. These benchmark tests were performed in this present study in order to validate the EDEM and PFC3D codes. The detailed description is given in Section 4.4.
Table 2.1 Summary of the literature review for benchmark tests

<table>
<thead>
<tr>
<th>Authors/Year</th>
<th>Methodology</th>
<th>Direction</th>
<th>Contact force model</th>
<th>Analysis</th>
<th>Compared methodology</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vu-Quoc &amp; Zhang, 1999a</td>
<td>DEM</td>
<td>Oblique impact</td>
<td>Bilinear spring system NFD model and improved TFD model</td>
<td>Normal: plastic; tangential: elastic friction</td>
<td>Dynamic principles</td>
</tr>
<tr>
<td>Kharaz et al., 2001</td>
<td>Experiment</td>
<td>Oblique impact</td>
<td></td>
<td>Normal: elastic; tangential: elastic friction</td>
<td>Dynamic principles and numerical results of Maw et al. (1976)</td>
</tr>
<tr>
<td>Zhang &amp; Vu-Quoc, 2002</td>
<td>FEA</td>
<td>Normal impact</td>
<td></td>
<td>Normal: elastic, elasto-perfectly plastic</td>
<td>Hertz theory and DEM with elasto-plastic NFD model (Vu-Quoc &amp; Zhang, 1999b)</td>
</tr>
<tr>
<td>Wu et al., 2003</td>
<td>FEA</td>
<td>Oblique impact</td>
<td></td>
<td>Normal: elasto-plastic; tangential: elasto-plastic friction</td>
<td>Dynamic principles, Hertz theory and numerical results of Maw et al. (1976)</td>
</tr>
<tr>
<td>Renzo &amp; Maio, 2004</td>
<td>DEM</td>
<td>Oblique impact</td>
<td>Linear spring model, Hertz-Mindlin no-slip model and complete Hertz-Mindlin model</td>
<td>Normal: elastic; tangential: elastic friction</td>
<td>Experiments of Kharaz et al. (2001) and numerical results of Maw et al. (1976)</td>
</tr>
</tbody>
</table>
2.3 Input parameters for DEM simulations

2.3.1 Young’s modulus and Poisson’s ratio

The Hertz contact theory has been widely used to determine the modulus of elasticity for various agricultural grains (Arnold and Roberts, 1969; Shelef and Mohsenin, 1969; Misra and Young, 1981; Jindal and Techasena, 1985). This determination is based on fitting the Hertz model to the force-displacement data from a single particle compression test and assuming a value of the Poisson’s ratio, as described in the ASAE Standard (1996). In this study, the ASAE indenter method was used initially but was found to be unsuitable for non-spherical particles which do not have sufficiently flat surfaces. A rigid platen compression test was then used to improve on the measurement. The detailed theoretical considerations and modulus measurements for the above two methods are presented in Section 5.3.1.

2.3.2 Friction coefficient

Several researchers have attempted to measure the friction coefficient, both particle-particle and particle-surface friction. Lorenz et al. (1997) calculated dynamic inter-particle friction coefficients for different types of material, such as polystyrene, stainless steel, acrylic and glass beads, by performing a binary collision experiment based on the Walton’s impact model. O’Sullivan et al. (2004a) presented a modified four-ball test to obtain static inter-particle friction coefficient for steel balls and conducted tilt tests to determine static friction coefficients between the steel balls and the boundary surface. However, almost all the research was limited to spherical or nearly spherical particles and may not be suitable for irregularly shaped particles, like corn grains and other cereal grains. On the other hand, Richter (1954) and Brubaker and Pos (1965) determined the particle-surface bulk friction coefficient of some agricultural materials using simple shear tests. Moya et al. (2002) measured the angle of internal friction for agricultural grains using the direct shear test. The literature on the measurement of individual friction coefficient for irregularly shaped particles is extremely limited. Individual particle-particle friction measurement has rarely been attempted before in irregularly shaped agricultural grains. In the present
study, the static particle-surface friction coefficients for irregularly shaped particles were estimated from a simple sliding test. The detailed theoretical considerations and experimental results for this method are described in Section 5.3.2.

2.3.3 Coefficient of restitution

The coefficient of restitution has been studied by many researchers. There are several different definitions proposed for the coefficient of restitution. These definitions are primarily classified as follows:

1. The normal restitution coefficient (Lorenz et al., 1997; Sharma and Bilanski, 1971; Gorham and Kharaz, 2000; Kharaz et al., 2001; Chau et al., 2002) is defined in terms of the normal components of the rebounding and incoming velocities, whilst the tangential restitution coefficient (Lorenz et al., 1997; Kharaz et al., 2001; Chau et al., 2002) is defined in terms of the tangential components of the rebounding and incoming velocities.

2. The resultant restitution coefficient (Chau et al., 2002; Yang and Schrock, 1994) is defined as the ratio of the rebounding velocity to the incoming velocity.

3. The energy restitution coefficient (LoCurto et al., 1997; Johnson, 1985) is defined in terms of the kinetic energies after and before impact.

Mishra (1991) calculated the normal coefficient of restitution for ball-ball collisions by the twin pendulum experiment. Lorenz et al. (1997) determined the normal and tangential restitution coefficients for different types of material such as polystyrene, stainless steel, acrylic and glass beads by performing binary collision experiments based on the Walton’s impact model. In their tests, the restitution coefficients for particle-particle collisions were obtained as well as the restitution coefficients for particle-surface collisions. In addition, the post collision spins were calculated based on the 2D rigid body theory. By means of highly accurate measurement of particle rebound characteristics, Gorham and Kharaz (2000) and Kharaz et al. (2001) evaluated the normal and tangential restitution coefficients for aluminium oxide spheres impacting a thick soda-lime glass anvil over impact angles from normal to very near glancing incidence. The accurate measurement was achieved by careful attention to all aspects of the experiment, including the mechanical and optical
systems, illumination, electronic control, computer-based image measurement and the geometry and condition of the impacting surfaces. The post collision spins were measured and compared with the simple theoretical model. Chau et al. (2002) applied a similar methodology (Lorenz et al., 1997; Gorham and Kharaz, 2000; Kharaz et al., 2001) to investigate rock fall impacts. However, all these studies focused only on spherical particles.

Most real particles, for example, agricultural grains, are not spheres. The literature concerning the coefficient of restitution for irregularly shaped particles is limited. LoCurto et al. (1997) determined the energy restitution coefficient for soybeans by conducting a simple drop test. In their experiments, only soybeans which rebounded with minimal rotation and with trajectories within (88.6° - 91.4°) range (inclination to the plate i.e. nearly vertical) were selected. The energy restitution coefficient was calculated according to the drop and rebound height. This is because it is possible for a proportion of these somewhat spherical soybeans to rebound nearly vertically so that the energy can be translated to the height of rebound. However, it is difficult to apply such test for irregularly shaped particles, since they will rebound randomly and very possibly with significant rotation. To date, only Yang and Schrock (1994) carried out a 3D analysis to acquire the normal and resultant restitution coefficients for irregularly shaped particles such as wheat, soybean, cheat, and goatgrass similarly using the drop test method. However they did not measure the rotational velocity after impact in their tests. The energy restitution coefficient was thus impossible to determine, as the rotational kinetic energy cannot be evaluated.

Table 2.2 shows a summary of the literature review for the coefficient of restitution, including main apparatus, objects, considered directions etc. It can be seen that none of these methods can be employed to determine the energy restitution coefficient for irregularly shaped particles. From the previous definitions, the energy restitution coefficient is a measure of the energy lost during a collision and should be explored for the force-displacement model necessary for the development of the discrete element method.
<table>
<thead>
<tr>
<th>Authors/Year</th>
<th>Directions</th>
<th>Objects</th>
<th>Plate material</th>
<th>Incident angle</th>
<th>Drop height (mm)</th>
<th>Main apparatus</th>
<th>Intended parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Yang et al., 1994</td>
<td>3-D</td>
<td>Wheat, soybean, cheat, goatgrass</td>
<td>Steel</td>
<td>0</td>
<td>No mention</td>
<td>Stroboscopic photography, image processing software</td>
<td>Resultant restitution coefficient</td>
</tr>
<tr>
<td>LoCurto et al., 1997</td>
<td>1-D</td>
<td>Soybean</td>
<td>Aluminium, glass, acrylic</td>
<td>0</td>
<td>151, 292, 511</td>
<td>High speed camera</td>
<td>Energy restitution coefficient</td>
</tr>
<tr>
<td>Lorenz et al., 1997</td>
<td>2-D</td>
<td>polystyrene, stainless steel, acrylic, glassbead</td>
<td>Aluminium</td>
<td>A range of angles</td>
<td>No mention</td>
<td>Stroboscopic photography, image processing software</td>
<td>Normal &amp; tangential restitution coefficient</td>
</tr>
<tr>
<td>Gorham &amp; Kharaz, 2000; Kharaz et al., 2001</td>
<td>2-D</td>
<td>Aluminium oxide sphere</td>
<td>Soda-lime glass, aluminium alloy</td>
<td>A range of angles</td>
<td>820</td>
<td>Stroboscopic photography, image processing software</td>
<td>Normal &amp; tangential restitution coefficient</td>
</tr>
<tr>
<td>Chau et al., 2002</td>
<td>2-D</td>
<td>Spherical boulders</td>
<td>Plaster slope</td>
<td>A range of angles</td>
<td>No mention</td>
<td>High speed camera</td>
<td>Normal &amp; tangential restitution coefficient</td>
</tr>
</tbody>
</table>

Table 2.2 Summary of the literature review for the coefficient of restitution
In the present study, the drop test method is extended to evaluate the energy restitution coefficient for any irregularly shaped particles. The method will also give the normal, tangential and resultant restitution coefficient by excluding certain measurements in the calculations. The rebounding linear and angular velocities at any instant is determined from the images taken using a high-speed camera. The 3D laser scanner is used to capture the three-dimensional surface geometry of the irregularly shaped test objects. The scanned data will be processed to determine the mass moments and products of inertia at any instant. The rotational kinetic energy together with translational kinetic energy can be evaluated, and the energy restitution coefficient can then be calculated. The results should facilitate the development of the contact model for irregularly shaped particles in DEM, and provide data for calibration and simple validation. The theoretical framework for this methodology and the details of the experimental apparatus are described in Section 5.3.3.

2.4 Contact force models

The particle-particle interaction greatly influences the kinematics of a particulate system and thus plays an important role. In DEM simulations, the Newton's second law of motion governing the mechanical behaviour of the particles are integrated numerically using a step-by-step procedure. Assume that the positions and velocities of all particles are given at time $t_{n-1}$. The task is to compute the forces and moments acting on each particle at $t_n$, and then to acquire the updated positions and velocities of all particles by integrating the Newton's second law of motion. Accordingly, it is important to correctly evaluate the contact forces between particles in collision.

There have been several contact force-displacement models for direct particle-particle collisions. Most of these force-displacement models for DEM simulations are based on the theories of contact mechanics.

Hertz (1896) proposed the normal force-displacement (NFD) relationship for spheres in contact and subjected to a normal force. Hertz theory provides a nonlinear elastic relationship between the contact normal displacement (overlap) and contact normal
force. When simulating a sphere colliding with a rigid flat surface, the coefficient of restitution is 1.0 using the Hertz theory. By adopting Hertz theory, Mindlin and Deresiewicz (1953) developed an incremental tangential force-displacement (TFD) relation for identical elastic spheres subjected to a frictional contact force in the tangential direction. The combined Hertz Mindlin no-slip contact model is commonly used in DEM simulations and is used throughout this thesis. It will be described in detail in the next chapter.

Energy dissipation occurs in most collision problems, thus making the coefficient of restitution less than one. To account for this behaviour, there are two approaches to dissipate the energy of the particulate system: damping and plastic deformation. Cundall and Strack (1979) presented a linear spring (Hooke's law) and dashpot model with a slider in which the dashpot (modelled by viscous damping) is used to account for the energy dissipation in the normal and tangential directions besides friction energy lost. Since this model is simple, direct and easy to implement, it is most widely used for DEM simulations. To improve the accuracy for the spring and dashpot model, Tsuji et al. (1992) proposed a nonlinear spring (Hertz theory) and dashpot model with a frictional slider in the tangential direction.

Walton and Braun (1986) used an alternative method to account for energy dissipation during contact and proposed a bilinear spring system NFD model for normal contact of spheres to account for plastic deformation and a simplified TFD model for elastic frictional contact. The bilinear spring system NFD model is based on finite element analysis (FEA) results and the simplified TFD model is an approximation of the Mindlin and Deresiewicz (1953) theory for the case of constant normal force during the change of the tangential force. To improve the accuracy for the tangential force calculation, Vu-Quoc and Zhang (1999a) developed an improved TFD model by incorporating into Walton and Braun's TFD model the four cases of varying normal forces and tangential forces from the Mindlin and Deresiewicz theory (1953). In their work, the NFD model still followed Walton's NFD model.

The coefficient of restitution was assumed to be a constant in the papers mentioned above. In reality, the coefficient of restitution decreases as the incoming velocity
increases, since the amount of plastic deformation increases, thus inducing more energy dissipation. Thornton (1997) presented an elasto-plastic NFD model that accounts for both elastic and plastic deformation in the normal direction and produces a coefficient of restitution for sphere collisions that decreases with increasing incoming velocity. However, the Thornton NFD model produces force-displacement curves that are too soft compared with the FEA results. Vu-Quoc and Zhang (1999b) also proposed an elasto-plastic NFD model that correctly accounts for the energy dissipation caused by the plastic deformation due to collisions. This model not only evaluates accurately the corresponding coefficient of restitution, but also gives force-displacement curves that are closer to the FEA results.

It should be pointed out that there is an inconsistency in the NFD model and the TFD model in the study proposed by Walton & Braun (1986) and Vu-Quoc & Zhang (1999a). Although the NFD model accounts for plastic deformation, the TFD model does not. To overcome this inconsistency, Vu-Quoc et al. (2001) developed elasto-plastic force-displacement models in both the normal direction and the tangential direction. This improved model is based on a frictional elasto-plastic finite element analysis of spheres in contact.

Table 2.3 shows the summary of the literature review for the contact force models. Although Thornton (1997) and Vu-Quoc et al. (2001) proposed better contact force models to account for plastic deformation during particle collisions and these models were also validated by FEA, it is not clear how to acquire the various particle properties needed to implement the model for a real solid, especially for agricultural grains that are inherently heterogeneous (agricultural grains being a focus in this thesis). In contrast, Tsuji et al. (1992) model only needs the Young’s modulus (shear modulus), Poisson’s ratio, friction coefficient and coefficient of restitution, which can be determined relatively easily in laboratory tests. In addition, this model is computationally relatively efficient and appears to give satisfactory numerical outcomes. Tsuji et al. (1992) model was therefore used for all DEM simulations in this study. An introduction of the Tsuji et al. (1992) model will be described in Section 3.2.
Table 2.3 Summary of the review for contact force models

<table>
<thead>
<tr>
<th>Authors/Year</th>
<th>Contact force model</th>
<th>Directions</th>
<th>Energy dissipation mechanism</th>
<th>Restitution coefficient</th>
<th>Consistency</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hertz, 1896</td>
<td>Elastic NFD model</td>
<td>Normal</td>
<td>No</td>
<td>1</td>
<td>NO</td>
</tr>
<tr>
<td>Mindlin &amp; Deresiewicz, 1953</td>
<td>Elastic TFD model</td>
<td>Tangential</td>
<td>No</td>
<td>Only friction</td>
<td>1</td>
</tr>
<tr>
<td>Cundall &amp; Strack, 1979</td>
<td>Linear spring &amp; dashpot model</td>
<td>Normal &amp; Tangential</td>
<td>Damping</td>
<td>Damping &amp; friction</td>
<td>Assumed to be constant</td>
</tr>
<tr>
<td>Walton &amp; Braun, 1986</td>
<td>Bilinear spring system NFD model and simplified TFD model</td>
<td>Normal &amp; Tangential</td>
<td>Plastic deformation</td>
<td>Only friction</td>
<td>Assumed to be constant</td>
</tr>
<tr>
<td>Tsuji et al., 1992</td>
<td>Nonlinear spring &amp; dashpot model</td>
<td>Normal &amp; Tangential</td>
<td>Damping</td>
<td>Damping &amp; friction</td>
<td>Assumed to be constant</td>
</tr>
<tr>
<td>Thornton, 1997</td>
<td>Elasto-plastic NFD model</td>
<td>Normal</td>
<td>Plastic deformation</td>
<td>As the incoming velocity increases, the restitution coefficient decreases</td>
<td>NO</td>
</tr>
<tr>
<td>Vu-Quoc &amp; Zhang, 1998a</td>
<td>Bilinear spring system NFD model and improved TFD model</td>
<td>Normal &amp; Tangential</td>
<td>Plastic deformation</td>
<td>Only friction</td>
<td>Assumed to be constant</td>
</tr>
<tr>
<td>Vu-Quoc &amp; Zhang, 1999b</td>
<td>Elasto-plastic NFD model</td>
<td>Normal</td>
<td>Plastic deformation</td>
<td>As the incoming velocity increases, the restitution coefficient decreases</td>
<td>NO</td>
</tr>
<tr>
<td>Vu-Quoc et al., 2001</td>
<td>Elasto-plastic NFD and elasto-plastic TFD model</td>
<td>Normal &amp; Tangential</td>
<td>Plastic deformation &amp; friction</td>
<td>As the incoming velocity increases, the restitution coefficient decreases</td>
<td>YES</td>
</tr>
</tbody>
</table>
2.5 Representation for non-spherical particles

Most particles in industrial applications are not spheres. In DEM simulations of granular media, representation of non-spherical particles is an important issue. The particle shape descriptor is crucial for an accurate simulation of real particle behaviour, with implications for contact detection algorithm and method for calculating contact forces, which in turn influence the computational efforts required for simulations.

In this study, the DEM simulations of several physical experiments are based on 3D computations, so we restrict our attention to the literature regarding 3D representation of non-spherical particles. There have been many methods for representing non-spherical particles. The descriptors can be categorised into five groups (Kremmer, 2001): (1) spheres; (2) ellipsoids; (3) multiple spheres; (4) continuous function representations; and (5) polyhedrons.

Spheres are the simplest and most common shape descriptor used to model the granular particles in 3D DEM simulations (Cundall, 1988; Walton et al., 1988; Thornton and Antony, 1998; many others). The contact detect algorithm and contact force resolution are simple, direct and computationally efficient, but spheres have an inherent tendency to rotate. As a result, angularity-induced dilation and particle interlocking are prevented. Thomas and Bray (1999) concluded that non-spherical particles exhibit a smaller tendency to rotate which results in higher shear strengths.

Ellipsoidal discrete elements were introduced by Lin and Ng (1995) and have been used in 3D DEM simulations by Lin and Ng (1997) and Ng (2001). Ellipsoids have a smaller tendency to rotate and the surface of ellipsoids is absolutely smooth by comparison with other descriptors (i.e. multiple spheres, continuous function representations and polyhedrons). However, the mathematical formulation is complex and contact detection is computationally intensive.

The multiple sphere descriptor for representing nonspherical particles with curved surfaces was proposed by Favier et al (1999) and a similar descriptor (named “clump
logic") has been incorporated into the commercial DEM software “Particle Flow Code PFC” (ITASCA, 1999). Any number of overlapping spheres can be fitted to the surface contour of a real particle. Contact detection and resolution are sphere-based and computationally effective, especially when the number of particles is huge. The main drawback is that the surface of represented particles may not be smooth or convex with limited overlapping spheres. This descriptor has been gaining popularity in 3D DEM simulations (Zhang and Vu-Quoc, 2000; Favier et al., 2001; Matsushima et al., 2003).

Irregularly shaped particles with curved surfaces can be represented by using one or more continuous functions to describe the surface contour. Hogue (1998) presented these shape representations and contact detection for 3D DEM simulations. Continuous function representations provide more flexibility for descriptions of convex and concave particles. However, the contact detection is significantly more computationally intensive due to the iteration required for solving nonlinear equations.

Polyhedron descriptor is designed to closely describe the shape of flat surfaced and angular particles, especially in rock mechanics. Liu and Lemos (2001) developed a contact resolution algorithm for block contact in 3D DEM models. This algorithm is only limited to modelling of six sided brick-shape discrete elements and is much more time-consuming than sphere-based algorithm.

Table 2.4 shows the comparisons for the five shape descriptors, including the advantages and disadvantages. It can be seen that for modelling the curved surface particles, like agricultural grains, and considering the computational efforts, the multiple sphere descriptor may be a good option. In the study, the multiple sphere method is adopted to represent the corn grains. An introduction of multiple sphere method will be described in Section 3.3.
### Table 2.4 Summary of the review of DEM particle shape descriptors

<table>
<thead>
<tr>
<th>Shape descriptor</th>
<th>Suitable shape</th>
<th>Advantages</th>
<th>Disadvantages</th>
<th>Authors/Year</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sphere</td>
<td>Only spheres</td>
<td>1. Contact detection and resolution are computationally efficient.</td>
<td>1. Spheres have an inherent tendency to roll, thus reducing their interlocking resistance.</td>
<td>Cundall, 1988; Walton et al., 1988; Thornton and Antony, 1998</td>
</tr>
<tr>
<td>Ellipsoid</td>
<td>Only ellipsoids</td>
<td>1. Ellipsoids have a smaller tendency to roll. 2. The surface of ellipsoids is absolutely smooth.</td>
<td>1. Mathematic formulation is complex. 2. Contact detection is computationally intensive.</td>
<td>Lin and Ng, 1995; Lin and Ng, 1997; Ng, 2001</td>
</tr>
<tr>
<td>Multiple sphere</td>
<td>Curved surface particles</td>
<td>1. Contact detection and resolution are sphere-based and computationally efficient. 2. Any number of overlapping spheres can be fitted to the surface contour of the real particle shape.</td>
<td>1. The surface of represented particles may be not smooth and convex with limited overlapping spheres.</td>
<td>Favier et al., 1999; Favier et al., 2001; Zhang and Vu-Quoc, 2000; PFC3D, 2003; Matsushima et al., 2003</td>
</tr>
<tr>
<td>Continuous function representation</td>
<td>Curved surface particles (convex and concave)</td>
<td>1. Representing the shape of convex and concave particles is more flexible.</td>
<td>1. Contact detection is more difficult due to the iteration for solving nonlinear equations.</td>
<td>Hogue, 1998</td>
</tr>
<tr>
<td>Polyhedron</td>
<td>Particles with edges and corners</td>
<td>1. Representing the shape of flat surfaced and angular particles is more close.</td>
<td>1. Polyhedrons may be not suitable for curved surface particles. 2. Contact detection is computationally intensive.</td>
<td>Liu and lemos, 2001</td>
</tr>
</tbody>
</table>
2.6 Experimental validation of the DEM

More recently, several researchers have validated their DEM results by conducting 3D DEM simulations and the corresponding physical tests. Most experimental validations came from laboratory tests in soil mechanics. The micro-mechanics underlying the observed macro-scale (bulk) response can be examined by reviewing these studies.

Zhang and Vu-Quoc (2000) simulated soybeans flowing down a bumpy inclined chute and the corresponding physical experiments were conducted. The 3D DEM simulations showed that the soybean flow developed from an unsteady state to a steady state flow. At the steady state flow, the average velocity of the granular flow calculated from the DEM simulations agreed with that from the corresponding experiments. On the boundary, the velocity profile from the simulations gave an agreement not only qualitatively, but also quantitatively with the experiments.

Odagí et al. (2002) performed 3D DEM simulations of compression test of zirconia-ceramic particles in a cylindrical die and compared with the corresponding experiments. Surface roughness of particles, measured using an atomic force microscope (AFM), was considered in the 3D DEM simulations. The study showed that the numerical results gave good agreement with experimental results for the relationship between the normalized pressure and axial strain.

Matsushima et al. (2003) validated simple shear tests of glass grains made by crushing blocks with 3D DEM simulations. The simple shear tests were conducted under constant confining pressure and under constant volume. The 3D irregular grain shapes were detected by a special visualization technique, called Laser-Aided Tomography. The multiple sphere method was used to represent the irregular shapes of the glass grains and the grain size distribution was also considered in the simulations. The study showed that the void ratios of specimens from the DEM simulations were 10% and 5% higher than those from the experiments for the densest and loosest situations, respectively. The DEM simulations also produced higher shear strength than the experiments.
O'Sullivan et al. (2004a) examined the triaxial and plane strain laboratory compression tests of steel spheres with face-centred-cubic and rhombic packings by conducting physical tests and 3D DEM simulations. The study showed that the 3D DEM simulations captured the peak strength values well in the triaxial and plane strain tests for both packing conditions. Nevertheless, the post-peak response is difficult to capture and is sensitive to the friction coefficients assumed between the steel spheres and boundaries.

O'Sullivan et al. (2004b) also examined the direct shear tests of stainless steel spheres by comparing physical tests and 3D DEM simulations. The study showed that the response from the DEM simulations was found to be significantly stiffer than that measured in the physical tests and the angle of internal friction from the simulations was also about 4.8° lower than that observed in the laboratory tests (mean value = 24.4°).

The literature regarding the experimental validation of the DEM is summarized in Table 2.5. Table 2.5 also indicates the contact force model, particle shape descriptor, number of particles and physical quantities obtained in these DEM simulations. In the present study, several calibration experiments including silo filling, confined compression, rod penetration and silo discharging were developed and conducted. The corresponding 3D DEM simulations were conducted and comparison between DEM simulations and experiments was made. Detailed description of the results is presented in Chapter 6.
Table 2.5 Summary for the review of experimental validation of DEM

<table>
<thead>
<tr>
<th>Field</th>
<th>Authors/Year</th>
<th>Contact force model</th>
<th>Particle shape descriptor</th>
<th>Number of particles</th>
<th>Physical quantity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chute flow of soybeans</td>
<td>Zhang and Vu-Quoc, 2000</td>
<td>Bilinear spring system NFD model and improved TFD model</td>
<td>Multiple sphere (One particle consists of 4 spheres)</td>
<td>1200</td>
<td>Average velocity of cross section, velocity profile</td>
</tr>
<tr>
<td>Compression test of zirconia-ceramic particles</td>
<td>Odagi et al., 2002</td>
<td>Hertz-Mindlin no slip model with a friction slider (no damping)</td>
<td>Sphere</td>
<td>35368</td>
<td>Normalized pressure - axial strain curve, contact force chain, contact orientation</td>
</tr>
<tr>
<td>Simple shear tests of crushed glass under constant confining pressure and constant volume</td>
<td>Matsushima, 2003</td>
<td>Linear spring and dashpot model</td>
<td>Multiple sphere (One particle consists of 10 spheres)</td>
<td>800</td>
<td>Void ratio, stress ratio - shear strain curve, volumetric strain - shear strain curve (dilation curve), stress ratio - vertical stress curve</td>
</tr>
<tr>
<td>Triaxial tests and plane strain tests of steel spheres</td>
<td>O'Sullivan et al., 2004a</td>
<td>Linear spring model (no damping)</td>
<td>Sphere</td>
<td>1512, 1519, 1944, 1953 for different cases</td>
<td>Angle of friction mobilized - axial strain curve</td>
</tr>
<tr>
<td>Direct shear tests of steel spheres</td>
<td>O'Sullivan et al., 2004b</td>
<td>Hertz-Mindlin no slip model with a friction slider (no damping)</td>
<td>Sphere</td>
<td>No mention</td>
<td>Horizontal strain-shear stress curve, peak shear stress-normal stress curve, local stresses, particle displacement, contact force chain, strain contours</td>
</tr>
</tbody>
</table>
2.7 Linking DEM and FEA

One method of evaluating the loading from particles interacting with a deformable body is to use the DEM outcomes for a FEA analysis. Cleary (1998) presented DEM simulations for the filling of dragline buckets and suggested that, by extracting data at small time intervals from the DEM simulation and spatially smoothing them, the time-varying dynamic load (pressure), acting on boundary surfaces of the dragline buckets, could be determined and used as input to an FEA analysis. Combined discrete element analysis and finite element analysis could be used to optimise the bucket design.

In this study, a methodology to link DEM with FEA was developed and this can be used to determine the stresses in the contacting body resulting from particle forces. The basic concepts and mathematic formulation for this methodology are described in Chapter 9.

2.8 Summary

The related literature regarding this study has been reviewed in this chapter. The literature includes benchmark tests for validating DEM codes, input parameters for DEM simulations, contact force models, representation for non-spherical particles, experimental validation of the DEM and linking DEM and FEA.
Chapter 3

Brief review of DEM

3.1 Introduction

The application of DEM to model the flow behaviour of a particle assembly requires cyclic calculations. In DEM, the equations of motion for the particles are integrated numerically using a step-by-step algorithm. The step-by-step integration procedure is typically as follows:

1. The positions and velocities of all particles are known at time $t_{n-1}$. The normal force and displacement for each contact are given and the tangential force and displacement for each contact are also given at time $t_{n-1}$.

2. The updated normal and tangential displacements at time $t_n$ are calculated over a small time step. The updated normal and tangential forces at time $t_n$ can then be evaluated according to the force-displacement contact model.

3. The forces and moments that act on each particle at time $t_n$ are summed.

4. The positions and velocities of all particles at time $t_n$ are calculated by integrating the equations of motion of particles numerically.

The above operations are repeated for each time step so that the motion of each particle can be determined. In this procedure there are several important aspects
including the contact force model, the representation of non-spherical particles, critical time step, contact detection, etc. In the present study, the Hertz-Mindlin with no slip contact model was used throughout to evaluate the normal and tangential contact forces. The multiple sphere method was employed to represent non-spherical particles. The determination of the computational time step is crucial for numerical stability and for keeping computing effort to a manageable level. The aim of this chapter is not to describe the DEM general methodology in details as this has been described many times before, but to discuss the key issues which are important for producing satisfactory numerical simulations. The DEM calculations in subsequent chapters were performed using both the EDEM code (DEM Solutions, 2005) and the PFC3D code (Itasca, 2003). The reason was to compare the outcomes of two independent DEM codes using exactly the same problem configurations.

3.2 Hertz-Mindlin with no slip contact model

Hertz-Mindlin no-slip contact model with damping and a frictional slider in the tangential direction, as shown schematically in Figure 3.1, is briefly reviewed in this section (Tsuji et al., 1992). This contact model is commonly used for DEM simulations and is available in PFC3D (ITASCA, 2003) and EDEM (DEM Solutions, 2005).
When sphere \( i \) is in contact with sphere \( j \), the normal component of the contact force, \( F_{CN} \), acting on sphere \( i \), is given by the sum of the normal spring force \( F_{CN,S} \) and normal damping force \( F_{CN,D} \) as

\[
F_{CN} = F_{CN,S} + F_{CN,D}
\] (3.1)

\( F_{CN,S} \) and \( F_{CN,D} \) are expressed in Eqs. (3.2) and (3.3), respectively. Eq. (3.2) is based on the Hertz contact theory and gives a nonlinear elastic relationship between the normal contact force and normal contact displacement.

\[
F_{CN,S} = -K_n \alpha_n^{3/2}
\] (3.2)

\[
F_{CN,D} = -2\sqrt{\frac{5}{6}} \beta_d \sqrt{m^* k_n} V_{relative,n}
\] (3.3)

where \( \alpha_n \) is the normal contact displacement (overlap), \( V_{relative,n} \) is the relative normal velocity (from sphere \( i \) to sphere \( j \)), and \( \beta_d \) is a damping ratio. The Hertz contact constant \( K_n \) is given by

\[
K_n = \frac{4G\sqrt{r^*}}{3(1-\nu)}
\] (3.4)
The normal contact stiffness \( k_n \) is given by

\[
k_n = \frac{2G}{(1-\nu)} \left[ \frac{3}{4} \frac{(1-\nu) r^* F_{CN,S}}{G} \right]^{1/3} \tag{3.5}
\]

where \( G \) is the shear modulus and \( \nu \) is the Poisson's ratio. The terms \( m^* \) and \( r^* \) are the equivalent mass and radius, and can be respectively expressed as

\[
m^* = \frac{m_i m_j}{m_i + m_j}, \quad r^* = \frac{r_i r_j}{r_i + r_j} \tag{3.6}
\]

where \( m_i \) and \( m_j \) denote the masses of sphere \( i \) and sphere \( j \), and \( r_i \) and \( r_j \) the radii of these spheres, respectively.

The tangential component of the contact force, \( F_{CT} \), is similarly given by the sum of the tangential spring force \( F_{CT,S} \) and tangential damping force \( F_{CT,D} \) as

\[
F_{CT} = F_{CT,S} + F_{CT,D} \tag{3.7}
\]

\( F_{CT,S} \) is normally expressed in incremental form as

\[
F_{CT,S} = F_{CT,S,(n-1)} + \Delta F_{CT,S} \tag{3.8}
\]

where \( F_{CT,S,(n-1)} \) is the spring force at the previous time step and \( \Delta F_{CT,S} \) is the increment of the tangential spring force. The increment \( \Delta F_{CT,S} \) is given by

\[
\Delta F_{CT,S} = k_i \Delta \alpha_i \tag{3.9}
\]
In Eq. (3.9), $k_t$ and $\Delta \alpha_t$ are the tangential contact stiffness and incremental tangential displacement, which can be expressed as Eqs. (3.10) and (3.11) respectively:

$$k_t = \frac{2}{(2-v)} \left[ 6(1-v)G^2 r^* F_{CN,S} \right]^{1/3} \tag{3.10}$$

$$\Delta \alpha_t = V_{\text{relative},t} \Delta t \tag{3.11}$$

where $V_{\text{relative},t}$ is the relative tangential velocity and $\Delta t$ is the time step.

The tangential damping force $F_{CT,D}$ is given by

$$F_{CT,D} = -2\sqrt{\frac{5}{6}} \beta_d \sqrt{m} k_t V_{\text{relative},t} \tag{3.12}$$

The tangential force is limited by the Coulomb-type friction law. That is, if the tangential force exceeds the maximum shear force allowed by the frictional slider, the tangential force is set equal to the maximum frictional value, as expressed in Eq. (3.13).

$$|F_{CT}| \leq \mu F_{CN,S} \tag{3.13}$$

Note that the limiting tangential force is a function of the normal spring force $F_{CN,S}$ only and not the total normal force $F_{CN}$ that includes the damping force. This was discovered to be necessary to match an analytical solution in one of the benchmark tests (Test No.6 in Section 4.4.6). Tangential force calculation in DEM is rather complex and often not clearly stated in the literature. It appears that PFC and EDEM codes both use Eq. (3.13).

The damping ratio $\beta_d$ is related to the coefficient of restitution $e$ and this relationship is given by (Tsuji et al., 1993)
\[ \beta_d = -\frac{\ln e}{\sqrt{(\ln e)^2 + \pi^2}} \] (3.14)

If the coefficient of restitution is regarded as a constant empirical parameter, the damping ratio may be determined from the above equation. It can be seen that the required parameters for this contact force model are the shear modulus (Young’s modulus), Poisson’s ratio, friction coefficient and coefficient of restitution. These parameters can be determined in the laboratory tests.

### 3.3 Multiple sphere method

In the DEM codes, PFC3D (ITASCA, 2003) and EDEM (DEM Solutions, 2005), the multiple sphere method is used to represent the shape of a non-spherical particle using a set of rigidly linked and inscribed element spheres. These spheres may be of different diameters and may overlap to any extent. They are placed at positions relative to the centre of gravity of the particle. The number, radii and positions of the spheres used to represent the particle govern the degree of approximation to the actual particle surface contour. The number of overlapping spheres depends on: (1) the degree of non-uniformity and angularity in the original particle shape, (2) the desired level of geometric accuracy, and (3) the computational time and resource limitation (Sallam et al., 2004).

In the multiple sphere method, contact detection between particles is sphere-based and any optimisation procedures developed for resolving sphere-sphere contact in DEM are completely applicable. The normal and tangential contact forces can then be calculated using standard discrete element formulation for spherical system. Contacts between these spheres inside the particle are skipped during the calculation cycle, resulting in a saving of computer time compared to a similar calculation in which all contacts are active. However, contacts with spheres external to the particle (from other particles) are not affected, i.e. such contacts will develop when the spheres comprising the boundary of the particle come into contact with other particles.
For completeness, the main equations for basic mass properties and motion for a non-spherical particle are given below. These equations are re-expressed in the vector form from the tensor form given in the PFC3D manual (ITASCA, 2003).

### 3.3.1 Mass, centroid and moment of inertia for a non-spherical particle

Consider a typical non-spherical particle consisting of \( N_s \) spheres, each of which has mass \( m_k \), radius \( r_k \) and centroid location \( \bar{x}_k \). The basic mass properties of the non-spherical particle are its total mass, \( m \), location of the mass centre, \( \bar{x}_G \), moments and products of inertial, \( I_{ij} \), and are defined by the following equations.

\[
m = \sum_{k=1}^{N_s} m_k \tag{3.15}
\]

\[
\bar{x}_G = \frac{1}{m} \sum_{k=1}^{N_s} m_k \bar{x}_k \tag{3.16}
\]

\[
I_{11} = \sum_{k=1}^{N_s} \left[ m_k (x_{k,2} - x_{G,2})^2 + m_k (x_{k,3} - x_{G,3})^2 + \frac{2}{5} m_k r_k^2 \right] \tag{3.17.a}
\]

\[
I_{22} = \sum_{k=1}^{N_s} \left[ m_k (x_{k,3} - x_{G,3})^2 + m_k (x_{k,1} - x_{G,1})^2 + \frac{2}{5} m_k r_k^2 \right] \tag{3.17.b}
\]

\[
I_{33} = \sum_{k=1}^{N_s} \left[ m_k (x_{k,1} - x_{G,1})^2 + m_k (x_{k,2} - x_{G,2})^2 + \frac{2}{5} m_k r_k^2 \right] \tag{3.17.c}
\]

\[
I_{12} = I_{21} = \sum_{k=1}^{N_s} \left[ m_k (x_{k,1} - x_{G,1})(x_{k,2} - x_{G,2}) \right] \tag{3.17.d}
\]

\[
I_{23} = I_{32} = \sum_{k=1}^{N_s} \left[ m_k (x_{k,2} - x_{G,2})(x_{k,3} - x_{G,3}) \right] \tag{3.17.e}
\]
The moments and products of inertia are defined with respect to a reference frame that is attached to the non-spherical particle at its mass centre $G_e$ and aligned with the global axis system. In general, this will be a non-principal set of axes (i.e. $I_y \neq 0$). It is noted that these equations for the basic mass properties is only an approximation when the element spheres overlap in a particle.

### 3.3.2 Equations of motion for a non-spherical particle

Since the spheres comprising a non-spherical particle remain at a fixed distance from each other, the non-spherical particle can be considered as a rigid body. The motion of the rigid body can be described in terms of the translational motion at the centre of mass $G_e$ and the rotational motion of the entire particle (Meriam and Kraige, 2003).

The translational motion of the non-spherical particle is described in term of its position ($\vec{x}_G$), velocity ($\dot{\vec{x}}_G$) and acceleration ($\ddot{\vec{x}}_G$) at the mass centre $G_e$, whilst the rotational motion is described in term of its angular velocity ($\vec{\omega}$) and angular acceleration ($\vec{\dot{\omega}}$). The equations for translational and rotational motions can be respectively expressed in the following vector forms.

\[
\vec{F} = m(\ddot{\vec{x}}_G - \vec{g}) \quad (3.18)
\]

\[
\vec{M}_G = \dot{\vec{H}} \quad (3.19)
\]

In Eq. (3.18), $\vec{F}$ is the resultant force vector, the sum of all contact forces acting on the particle, $m$ is the total mass of the particle, and $\vec{g}$ is the gravity acceleration vector. In Eq. (3.19), $\vec{M}_G$ is the resultant moment vector taken about the mass centre $G_e$ and $\dot{\vec{H}}$ is the time rate of change of the angular momentum about the mass centre. The angular momentum $\vec{H}$ can be given in matrix form by
\{ H \} = [ I_{\text{inertia}} ] \{ \omega \} \quad (3.20)

where \( \{ H \}^T = \{ H_1 \ H_2 \ H_3 \} \) and \( \{ \omega \}^T = \{ \omega_1 \ \omega_2 \ \omega_3 \} \). \( I_{\text{inertia}} \) is called the inertia tensor or inertia matrix and is written as

\[
[I_{\text{inertia}}] = \begin{bmatrix}
I_{11} & -I_{12} & -I_{13} \\
-I_{21} & I_{22} & -I_{23} \\
-I_{31} & -I_{32} & I_{33}
\end{bmatrix} \quad (3.21)
\]

Eq. (3.18) relates the resultant force to the translational motion and Eq. (3.19) relates the resultant moment to the rotational motion. The motion of the non-spherical particle is determined by the resultant force and moment vectors acting upon it.

The resultant force and moment resulting from the contact forces are respectively calculated by

\[
\vec{F} = \sum_{k=1}^{N_s} \sum_{l=1}^{N_{c,k}} \vec{F}_{k,l} \quad (3.22)
\]

\[
\vec{M}_G = \sum_{k=1}^{N_s} \sum_{l=1}^{N_{c,k}} (\vec{x}_{c,l} - \vec{x}_G) \times \vec{F}_{k,l} \quad (3.23)
\]

where \( N_s \) is the number of the spheres comprising the non-spherical particle and \( N_{c,k} \) is the number of contact in each sphere. In Eq. (3.22), \( \vec{F}_{k,l} \) is the force acting on particle \( k \) at contact \( l \). In Eq. (3.23), \( \vec{x}_{c,l} \) is the position vector of contact point on particle \( k \) at contact \( l \) and the symbol "\( \times \)" means the vector cross product.

Eq. (3.19) is written with respect to a local coordinate system that is attached to the non-spherical particle at its mass centre. For such a system, the time rate of change of the angular momentum \( \dot{H} \) can be written as

33
The equations of motions (Eqs. 3.18 and 3.19) can be integrated using a central finite difference procedure. Considering a time step of $\Delta t$, the quantities $\dot{x}$ and $\dot{\omega}$ are computed at the mid-intervals of $t \pm \Delta t / 2$ and the other quantities $x, \ddot{x}, \dot{\omega}, F$ and $\tilde{M}_G$ are computed at the primary intervals of $t \pm \Delta t$. The translational and rotational accelerations at time $t$ in terms of the velocity values at mid-intervals are expressed in the following finite difference expressions.

\[ \ddot{x}_t = \frac{1}{\Delta t} (\dot{x}_{t+\Delta t/2} - \dot{x}_{t-\Delta t/2}) \]  
\[ \ddot{\omega}_t = \frac{1}{\Delta t} (\dot{\omega}_{t+\Delta t/2} - \dot{\omega}_{t-\Delta t/2}) \]

Substituting Eq. (3.25) into Eq. (3.18) and rearranging for the velocity at time $t + \Delta t / 2$ gives

\[ \dot{x}_{t+\Delta t/2} = \dot{x}_{t-\Delta t/2} + \left( \frac{\vec{F}}{m} + \vec{g} \right) \Delta t \]  

Obtaining the angular velocity at time $t + \Delta t / 2$ requires solving a set of nonlinear equations using an iterative procedure during each time step. Substituting Eq. (3.24) into Eq. (3.19) results in

\[ \{M_G\} - \{W\} = \{I\}\{\dot{\omega}\} \]  

where $\{M_G\}^T = \{M_1 \ M_2 \ M_3\}$, $\{\dot{\omega}\}^T = \{\dot{\omega}_1 \ \dot{\omega}_2 \ \dot{\omega}_3\}$ and
\[ \{W\} = \begin{bmatrix} \omega_2 \omega_3 (I_{33} - I_{22}) + \omega_3 \omega_2 I_{23} - \omega_2 \omega_3 I_{32} - \omega_1 \omega_2 I_{31} + \omega_1 \omega_3 I_{21} \\ \omega_3 \omega_1 (I_{11} - I_{33}) + \omega_1 \omega_3 I_{31} - \omega_3 \omega_1 I_{13} - \omega_2 \omega_3 I_{12} + \omega_2 \omega_1 I_{32} \\ \omega_1 \omega_2 (I_{22} - I_{11}) + \omega_2 \omega_1 I_{12} - \omega_1 \omega_2 I_{21} - \omega_3 \omega_1 I_{23} + \omega_3 \omega_2 I_{13} \end{bmatrix} \] (3.29)

Eq. (3.28) provides three equations for the six unknowns, \( \{\omega\} \) and \( \{\dot{\omega}\} \). These six unknowns are determined by using the following iterative procedures.

1. Set \( n = 0 \).
2. Set \( \ddot{\omega}_0 \) equal to the initial angular velocity (i.e. before the motion computation).
3. Solve Eq. (3.28) for \( \ddot{\omega}_n \).
4. Determine a new angular velocity.
   \[ \ddot{\omega}_{\text{new}} = \ddot{\omega}_0 + \ddot{\omega}_n \Delta t \] (3.30)
5. Revise the estimate of \( \ddot{\omega} \) as
   \[ \ddot{\omega}_{n+1} = (\ddot{\omega}_0 + \ddot{\omega}_{\text{new}})/2 \] (3.31)
6. Go to Step 3 and repeat Step 4 and 5.

Numerical experimentation has shown that the iteration tends to converge after a few iterations (say 4 iterations). After four iterations have been performed, we set \( \ddot{\omega} = \ddot{\omega}_4 \).

After determining the translational and rotational velocities of the non-spherical particle, the position of the mass centre is updated by Eq. (3.32).

\[ \tilde{x}_{G,t+\Delta t} = \tilde{x}_{G,t} + \dot{\tilde{x}}_{G,t+\Delta t/2} \Delta t \] (3.32)

The velocity of each sphere in the non-spherical particle is determined by Eq. (3.33). The position of each sphere in the non-spherical particle is then updated based on the
position of the mass centre $G_e$ (Eq. 3.32) and the fixed relative position between the mass centre of each sphere and the mass centre of the particle $G_e$.

$$\dot{\mathbf{x}}_k = \dot{\mathbf{x}}_G + \mathbf{ω} \times (\mathbf{x}_k - \mathbf{x}_G)$$ \hspace{1cm} (3.33)

### 3.4 Determination of computational time step

In general, DEM usually employs the explicit and central time-finite-difference scheme. Although this explicit numerical scheme is more computationally efficient than the implicit numerical scheme, there is a limitation that it is only conditionally stable, so small time steps must be used. If the used time step is greater than a critical time step, the scheme is unstable and the simulation outcomes are unreliable.

In an assembly of particles, the force transmission between individual particles is through the Rayleigh wave that travels around the surface of elastic bodies. The criterion to determine a time step for DEM simulations is that the time step for calculating the incremental forces and displacements must be less than the time it takes for the wave to transverse the minimum size particle in the assembly. The Rayleigh wave velocity of force transmission is given by (Johnson, 1985)

$$V_R = \chi \sqrt{\frac{G}{\rho}}$$ \hspace{1cm} (3.34)

where $G$ and $\rho$ are the shear modulus and density of the particles respectively; $\chi$ is a function of the Poisson’s ratio $\nu$ and can be approximately expressed as (Thornton and Randall, 1988)

$$\chi = 0.1631\nu + 0.8766$$ \hspace{1cm} (3.35)

Provided that the properties of all constituent particles are the same, the critical time step $\Delta t_c$ is therefore given by
where \( r_{\text{min}} \) is the radius of the minimum size particle in the assembly. For an assembly consisting of different material type particles, the critical time step should be the smallest among those determined by different material properties.

For PFC DEM code, Itasca (2003) presented a simple method to estimate the critical time step for an assembly of particles using an equivalent single degree of freedom system. By considering the system to be an infinite series of point masses and springs (as shown in Figure 3.2) and based on the natural frequency concept, the critical time step is expressed as

\[
\Delta t_c = \frac{\pi \cdot r_{\text{min}} \sqrt{\rho}}{K} \sqrt{G}
\]  

(3.36)

where \( K \) is the contact spring stiffness and \( m \) is the particle mass.

It is interesting to note that the difference by using Eq. (3.36) and Eq. (3.37) for calculating the critical time step is not large. For example, consider the glass bead assembly with a sphere radius of 10 mm and the material properties as follows: Young’s modulus = 48 GPa; Poisson’s ratio = 0.2; density = 2800 kg/m\(^3\). Figure 3.3 shows the critical time step versus strain for the above two formulas. In Figure 3.3, the strain is defined as the ratio of the maximum overlap to the sphere radius and the contact spring stiffness \( K_{\text{contact}} \) in Eq. (3.37) is set simply to the secant stiffness \( \frac{F_{n,\text{max}}}{\alpha_{n,\text{max}}} \) (the ratio of the maximum normal contact force to the maximum

\[
\Delta t_c = \sqrt{\frac{m}{K_{\text{contact}}}}
\]  

(3.37)

Figure 3.2 Multiple mass-spring system (redrawn from Itasca, 2003)
It can be seen that the difference of the critical time step varies between \(-0\%\) and \(-40\%\) for up to 10\% strain.

**Figure 3.3** Critical time step versus strain for two different methods

It should be noted that Eq. (3.36) and Eq. (3.37) are the simplified formulas for estimating the critical time step. The actual computation time step used in DEM simulations is normally chosen by multiplying the critical time step with a fraction. Zhang (2003) proposed that this fraction should normally be less than 0.5 depending on the problems considered. Itasca (2003) suggested that the critical time increment should be multiplied by a safety factor with a default value of 0.8. DEM Solutions (2005) suggested a multiplier for the critical time step with a default value of 0.4.

O'Sullivan and Bray (2004c) proposed an approach to calculate the computation time step for the response of uniform spheres with regular packing arrangements. This method was based on a direct analogy between the nodes and elements of a finite element and contacts of a discrete element assembly. The contact element mass and stiffness matrices were formed considering different packing configurations and if the rotation is included. The critical time step was then calculated using an eigenvalue procedure. Figure 3.4 shows the critical time steps for various configurations of uniform spheres. The last two sphere arrangements in the first
column of Figure 3.4 are face-centred-cubic packing and rhombic packing respectively.

It can be seen from Figure 3.4 that if the particle mass is distributed equally amongst all contacts, the minimum critical time step is $\sqrt{\frac{1}{6} \frac{m}{K}}$ (i.e. $0.408\sqrt{\frac{m}{K}}$) for the case of translational motion only and the minimum critical time step is $\sqrt{\frac{1}{15} \frac{m}{K}}$ (i.e. $0.258\sqrt{\frac{m}{K}}$) when rotational motion is also considered. If the particle mass is distributed in a non-uniform manner, then the minimum critical time step is $0.348\sqrt{\frac{m}{K}}$ for translation only, and the minimum critical time step is $0.221\sqrt{\frac{m}{K}}$ for translation and rotation. Consequently, for the three-dimensional cases with uniform-sized spheres, the critical time step should be less than $0.221\sqrt{\frac{m}{K}}$ if rotation is allowed and $0.348\sqrt{\frac{m}{K}}$ if rotation is not allowed (O'Sullivan and Bray, 2004c). The study showed that the critical time step for an assembly was a function of the packing configuration and number of contacts per particle (the coordination number). As the coordination number increases, the critical time step decreases.

In the present study, a multiplier for critical time step (Eq. 3.36) was set equal to 0.01 (1%) in the simulations for all benchmark tests in Chapter 4, whilst a multiplier of 0.20 (20%) was chosen for all DEM simulations of physical experiments in Chapter 6, the sensitivity analyses in Chapter 7 and the analyses of gravity effect in Chapter 8. The value of 20% was chosen to balance computational accuracy with computational speed.
<table>
<thead>
<tr>
<th>Sphere Arrangement</th>
<th>$\Delta t_{\text{crit}}$ Translation</th>
<th>$\Delta t_{\text{crit}}$ Translation + Rotation</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1" alt="Sphere Arrangement 1" /></td>
<td>$\sqrt{\frac{1}{2}} \sqrt{\frac{m}{K}}$</td>
<td>$\sqrt{\frac{1}{3}} \sqrt{\frac{m}{K}}$</td>
</tr>
<tr>
<td><img src="image2" alt="Sphere Arrangement 2" /></td>
<td>$\sqrt{\frac{2}{3}} \sqrt{\frac{m}{K}}$</td>
<td>$\sqrt{\frac{2}{5}} \sqrt{\frac{m}{K}}$</td>
</tr>
<tr>
<td><img src="image3" alt="Sphere Arrangement 3" /></td>
<td>$\sqrt{\frac{1}{3}} \sqrt{\frac{m}{K}}$</td>
<td>$\sqrt{\frac{1}{5}} \sqrt{\frac{m}{K}}$</td>
</tr>
<tr>
<td><img src="image4" alt="Sphere Arrangement 4" /></td>
<td>$\sqrt{\frac{1}{6}} \sqrt{\frac{m}{K}}$ **</td>
<td>$\sqrt{\frac{1}{15}} \sqrt{\frac{m}{K}}$ **</td>
</tr>
<tr>
<td><img src="image5" alt="Sphere Arrangement 5" /></td>
<td>0.374 $\sqrt{\frac{m}{K}}$ **</td>
<td>0.297 $\sqrt{\frac{m}{K}}$ **</td>
</tr>
<tr>
<td><img src="image6" alt="Sphere Arrangement 6" /></td>
<td>0.348 $\sqrt{\frac{m}{K}}$ **</td>
<td>0.221 $\sqrt{\frac{m}{K}}$ **</td>
</tr>
</tbody>
</table>

Note: The solid line indicates the contact element considered in the calculations.
* Uniform distribution of inertia values to contact elements; ** Non-uniform distribution of inertia values to contact elements

**Figure 3.4** Critical time steps for various configurations of uniform spheres (cited from O'Sullivan and Bray, 2004c)
3.5 Summary

A brief review of the DEM has been given in this chapter including a step-by-step outline of the numerical procedure normally used in DEM codes. Several key issues that are important for achieving satisfactory DEM predictions have been discussed. These include the Hertz-Mindlin with no slip contact model that is used throughout in this thesis, the multiple sphere method for representing non-spherical particles and the determination of the computational time step.

For the critical time step, it has been shown that the Rayleigh wave concept (Eq. 3.36) and the natural frequency concept (Eq. 3.37) for calculating the critical time step both gave comparable outcomes. The study of O’Sullivan and Bray (2004c) showed that the critical time step is a function of the packing condition and coordination number, and for 3D uniform-sized spheres, it should be less than $0.22\sqrt{m/K}$. It is suggested that this provides a sound reference value for the computational time step in DEM simulations and a multiplier of 20% is appropriate. Choosing a multiplier that is larger than 20% speeds up the calculation but may lead to increasing numerical inaccuracy.
Chapter 4

Benchmark tests for validating DEM codes

4.1 Introduction

Discrete element method simulates the dynamics of each particle in an assembly by calculating the acceleration resulting from all the contact forces. It is clearly necessary that such a model is validated by comparing with experimental results, analytical solutions or other numerical results (e.g. FEA). DEM is now very widely used to model a very wide range of granular flow problems but looking at the literature, it is far from clear whether the large number of DEM codes have been validated and checked against benchmark problems. There appears to be no standard benchmark tests against which DEM codes can be validated. It was deemed necessary that the two DEM codes used in this thesis are first validated for simple cases to make sure that the codes are modelling the particle dynamics properly. This chapter describes the background and results of the benchmark tests conducted.

The chapter first describes analytical solutions regarding the elastic normal collision of two spheres or a sphere impacting on a rigid flat wall. The analytical solutions regarding the oblique collision are then derived and presented. A set of benchmark tests for validating spherical contact are subsequently presented. These benchmark tests not only validate the DEM codes but have also enhanced the understanding of
fundamental impact phenomena. They are also preliminary simulations for modelling physical experiments consisting of tens of thousands of particles.

4.2 Analytical solutions for elastic normal impact

Consider elastic impact of two identical spheres with no spin along the line joining their centres, as shown in Figure 4.1. Let $V_1$ and $V_2$ be the incoming velocities of Sphere 1 and Sphere 2 respectively. The relative velocity for this approach is expressed by

$$V_{\text{relative}} = V_1 + V_2$$  \hfill (4.1)

The force-displacement relation during the collision can be described using the Hertz contact theory. The solution for the elastic normal impact can be found in Timoshenko and Goodier (1970). The duration of the collision is given by

$$t_{\text{duration}} = 2.943 \left[ \frac{5\sqrt{2} \pi \rho (1 - \nu^2)}{4 E} \right]^{\frac{2}{5}} \frac{r}{V_{\text{relative}}^{1/5}}$$  \hfill (4.2)

where $E$ is the Young’s modulus, $\nu$ is the Poisson’s ratio, $\rho$ is the density, and $r$ is the radius of the two spheres. The maximum normal contact displacement and contact force are respectively

$$\alpha_{\text{max}} = \left[ \frac{5\sqrt{2} \pi \rho (1 - \nu^2) V_{\text{relative}}^2}{4 E} \right]^{\frac{2}{5}} r$$  \hfill (4.3)

$$P_{\text{max}} = \left[ \frac{2}{9} \frac{r E^2}{(1 - \nu^2)^2} \right]^{\frac{1}{2}} \alpha_{\text{max}}^3$$  \hfill (4.4)
Eqs. (4.2-4.4) can also apply to the case where a sphere impacts a rigid planar surface normally. Consider two spheres colliding with the same and opposite velocity as shown in Figure 4.2: since the contact of the spheres pressed against each other is symmetrical, this case is equivalent to the case where a sphere impacts on a rigid surface. For a sphere impacting on a rigid plane with incoming velocity $V_1$, the contact duration, maximum normal contact displacement and contact force are respectively

\[
t_{\text{duration}} = 2.943 \left[ \frac{5 \sqrt{2} \pi \rho (1 - v^2)}{4 \ E} \right]^2 \frac{r}{(2V_1)^{1/5}} \tag{4.5}
\]

\[
\alpha_{\text{max}} = \frac{1}{2} \left[ \frac{5 \sqrt{2} \pi \rho (1 - v^2)(2V_1)^2}{4 \ E} \right]^{2/5} r \tag{4.6}
\]

\[
P_{\text{max}} = \left[ \frac{2 \ rE^2}{9 (1 - v^2)^2} \right]^2 \left[ \frac{5 \sqrt{2} \pi \rho (1 - v^2)(2V_1)^2}{4 \ E} \right]^{2/5} r \tag{4.7}
\]
4.3 Analytical solutions for oblique impact

The problem of hard-sphere collisions with friction was presented by Vu-Quoc and Zhang (1999a) and employed as a benchmark test to validate the tangential force calculation. The analytical solutions obtained from dynamics principles for oblique impact were reviewed here in more details.

Consider an oblique impact between two homogeneous spheres in a 3D space, as illustrated in Figure 4.3. \( m_1 \) and \( m_2 \) denote the masses of Sphere 1 and Sphere 2, \( r_1 \) and \( r_2 \) the radii, and \( I_1 \) and \( I_2 \) the mass moments of inertia of these spheres about their centres of mass, respectively. Let \( \vec{V}_1 \) and \( \vec{V}_2 \) be the pre-collision linear velocities at their centres of mass, and \( \vec{\omega}_1 \) and \( \vec{\omega}_2 \) the pre-collision angular velocities of these spheres, respectively. The two spheres are colliding at the contact point \( C \).

The relative velocity of Sphere 1 with respect to Sphere 2 at the contact point is given by

\[
\vec{V}_{cp,21} = \vec{V}_1 - \vec{V}_2 - \vec{\omega}_1 \times r_1 \vec{n} - \vec{\omega}_2 \times r_2 \vec{n}
\]  

(4.8)
where $\vec{n}$ is the unit normal vector joining the centre of Sphere 2 to the centre of Sphere 1 at contact. The unit normal vector, $\vec{\lambda}$, of the plane where the normal and tangential contact forces occur is expressed as

$$\vec{\lambda} = \frac{\vec{V}_{cp,21} \times \vec{n}}{|\vec{V}_{cp,21} \times \vec{n}|} \quad (4.9)$$

Figure 4.3 A schematic of two colliding spheres in a 3D Cartesian coordinate system

The unit vector for the tangential direction can then be expressed as

$$\vec{t} = \vec{n} \times \vec{\lambda} \quad (4.10)$$

An orthogonal coordinate system, based on the three unit vectors $\vec{t}$, $\vec{n}$ and $\vec{\lambda}$, can be established, as shown in Figure 4.4. The linear and angular velocities immediately before and after impact can be decomposed into components along the $\vec{t}$, $\vec{n}$ and $\vec{\lambda}$ directions using coordinate transformation. Figure 4.4 also depicts the pre-collision and post-collision linear and angular velocities. For Sphere 1, $V_{cn,1}$ and $V_{ct,1}$ denote the pre-collision normal velocity and tangential velocity at its centre of
mass, $V_{st,1}$ the pre-collision tangential velocity at the contact point and $\omega_1$ the pre-collision angular velocity, whilst $V'_{cn,1}$ and $V'_{ct,1}$ denote the post-collision normal and tangential velocity, $V'_{st,1}$ the post-collision tangential velocity, and $\omega'_1$ the post-collision angular velocity respectively. Similar notations also apply to Sphere 2.

![Diagram of spheres with velocities](image)

**Figure 4.4** Linear and angular velocities before and after impact in an orthogonal coordinate system based on $\vec{r}$, $\vec{n}$, and $\vec{l}$

Figure 4.5 illustrates the normal contact force $f_n$ and tangential contact force $f_t$ in a free-body diagram during impact. Considering homogeneous spheres and applying the linear and angular impulse-momentum principles to Sphere 1, three impulse-momentum equations can be expressed as

\[
F_t = \int_0^T f_t \, dt = -m_1 (V'_{ct,1} - V_{ct,1}) \tag{4.11}
\]

\[
F_n = \int_0^T f_n \, dt = m_1 (V'_{cn,1} - V_{cn,1}) \tag{4.12}
\]

\[
r_1 F_t = -I_1 (\omega'_1 - \omega_1) \tag{4.13}
\]
where \( T \) is the contact duration, \( F_n \) is the normal linear impulse and \( F_t \) is the tangential linear impulse. Similarly, another three impulse-momentum equations for Sphere 2 can be written as

\[
F_t = m_2 (V_{ct,2} - V_{ct,2}) \tag{4.14}
\]

\[
F_n = -m_2 (V_{cn,2} - V_{cn,2}) \tag{4.15}
\]

\[
r_2 F_t = -I_2 (\omega_2' - \omega_2) \tag{4.16}
\]

![Free body diagram](image)

**Figure 4.5** Normal and tangential contact forces during impact

The relative normal velocities immediately before and after impact can be expressed in Eqs. (4.17-4.18). The relative tangential velocities at the centre of mass immediately before and after impact can be expressed in Eqs. (4.19-4.20). The relative tangential velocities at the contact point immediately before and after impact can be expressed in Eqs. (4.21-4.22).

\[
V_{cn} = V_{cn,1} - V_{cn,2} \tag{4.17}
\]
\[ V_{cn}' = V_{cn,1}' - V_{cn,2}' \]  
(4.18)

\[ V_{ct} = V_{ct,1} - V_{ct,2} \]  
(4.19)

\[ V_{ct}' = V_{ct,1}' - V_{ct,2}' \]  
(4.20)

\[ V_{st} = V_{st,1} - V_{st,2} \]  
(4.21)

\[ V_{st}' = V_{st,1}' - V_{st,2}' \]  
(4.22)

The relationships between the tangential velocities at the contact point and those at the centre of mass can be written as

\[ V_{st,1} = V_{ct,1} + r_1 \omega_1 \]  
(4.23)

\[ V_{st,2} = V_{ct,2} - r_2 \omega_2 \]  
(4.24)

\[ V_{ct,1}' = V_{ct,1}' + r_1 \omega_1' \]  
(4.25)

\[ V_{ct,2}' = V_{ct,2}' - r_2 \omega_2' \]  
(4.26)

Now, let us define the normal coefficient of restitution as

\[ e_n = \frac{V_{cn}'}{V_{cn}} \]  
(4.27)

The tangential coefficients of restitution based on the centre of mass and contact point are defined respectively as

\[ e_t = \frac{V_{ct}'}{V_{ct}} \quad \beta = \frac{V_{st}'}{V_{st}} \]  
(4.28)
Combining Eqs. (4.12), (4.15), (4.17) and (4.18) together with Eq. (4.27) yields

\[ F_n \left( \frac{1}{m_1} + \frac{1}{m_2} \right) = -(1 + e_n) V \varepsilon \]  \hspace{2cm} (4.29)

Similarly, combining Eqs. (4.11), (4.14), (4.19) and (4.20) together with Eq. (4.28) for \( e_i \) yields

\[ F_i \left( \frac{1}{m_1} + \frac{1}{m_2} \right) = (1 - e_i) V \varepsilon \]  \hspace{2cm} (4.30)

Similarly, combining Eqs. (4.11), (4.14) and (4.23-4.26) together with Eqs. (4.21), (4.22) and (4.28) for \( \beta \) yields

\[ F_i \left( \frac{1}{m_1} + \frac{1}{m_2} \right) = (1 + \beta) V_{st} + r_1 (\omega_{1}' - \omega_{1}) + r_2 (\omega_{2}' - \omega_{2}) \]  \hspace{2cm} (4.31)

Further, combining Eqs. (4.13) and (4.16) into Eq. (4.31) and replacing \( I_1 \) and \( I_2 \) with \( \frac{2}{5} m_1 r_1^2 \) and \( \frac{2}{5} m_2 r_2^2 \) result in

\[ F_i \left( \frac{1}{m_1} + \frac{1}{m_2} \right) = \frac{2}{7} (1 + \beta) V_{st} \]  \hspace{2cm} (4.32)

There are two regimes, sliding regime and sticking regime, for this hard-sphere collision problem. They may arise depending on the incident angle, \( \tan^{-1}(V_{st}/V_{\varepsilon}) \), at the contact point. Consider the two cases of sliding collision and sticking collision:

(1) Sliding regime: The two spheres slide at the contact point during the collision. The Coulomb friction law should be satisfied, as expressed in Eq. (4.33).

\[ |f_i| = \mu f_n \]  \hspace{2cm} (4.33)
where \( \mu \) is the coefficient of sliding friction for the two spheres at contact. Eq. (4.33) is also equivalent to Eq. (4.34).

\[ |F_t| = \mu F_n \]  
\[ (4.34) \]

Provided that \( V_{st} > 0 \), substituting Eqs. (4.29-4.30) into Eq. (4.34), the relationship between \( e_t, e_n, \mu \) and \( \frac{V_{ct}}{V_{cn}} \) can be derived as

\[ (1-e_t)\frac{V_{ct}}{V_{cn}} + \mu(1+e_n) = 0 \]  
\[ (4.35) \]

Similarly, substituting Eqs. (4.29) and (4.32) into Eq. (4.34), the relationship between \( \beta, e_n, \mu \) and \( \frac{V_{cn}}{V_{st}} \) can be derived as

\[ \frac{2}{7} \frac{(1+\beta) V_{st}}{(1+e_n) V_{cn}} + \mu = 0 \]  
\[ (4.36) \]

From Eqs. (4.35-4.36), it can be seen that once the normal restitution coefficient \( e_n \), friction coefficient \( \mu \) and pre-collision velocities are given, the tangential restitution coefficients, \( e_t \) and \( \beta \), can be determined in the sliding regime. The relationship between \( e_t \) and \( \beta \) can also be obtained as Eq. (4.37) by combining Eqs. (4.35-4.36).

\[ (1-e_t)V_{ct} = \frac{2}{7}(1+\beta)V_{st} \]  
\[ (4.37) \]

Recalling Eq. (4.28) for \( \beta \), Eq. (4.36) can be rearranged and expressed as

\[ -\frac{V_{st}'}{V_{cn}} = \frac{7}{2} \mu \frac{1}{e_n} + \frac{1}{e_n} \frac{V_{st}}{V_{cn}} \]  
\[ (4.38) \]
The above equation describes the relationship between the tangent of incident angle, \( \frac{V_{st}}{V_{cn}} \), and the tangent of recoil angle, \( \frac{V'_{st}}{V'_{cn}} \), for sliding collision. This equation will be used in the benchmark testing in the next section.

(2) Sticking regime: Due to no sliding between the two spheres during the collision, the following relation must be followed.

\[
|F_t| < \mu F_n
\]  

(4.39)

Similar to the derivation of Eqs. (4.35-4.36), we have the following inequality for a stick collision provided that \( V_{st} > 0 \).

\[
(1 - e_t) \frac{V_{st}}{V_{cn}} + \mu(1 + e_n) > 0
\]  

(4.40)

\[
\frac{2 (1 + \beta) V_{st}}{7 (1 + e_n) V_{cn}} + \mu > 0
\]  

(4.41)

It should be noted that Eqs. (4.35-4.38) and (4.40-4.41) can be applied to the case where a sphere obliquely impacts on a rigid surface, as shown in Figure 4.6. As for the situation that \( V_{st} < 0 \), following the same derivation and noting that the tangential force, \( f_t \), is always opposite to the relative pre-collision tangential velocity at the contact point, \( V_{st} \), the corresponding equations can also be obtained. These equations will not be described here.
4.4 Benchmark tests

A set of benchmark tests has been set up to validate the DEM codes, as summarized in Table 4.1. Test No.1 and Test No.2 (Timoshenko and Goodier, 1970) were conducted to check the elastic normal contact of two identical spheres and of a sphere with a rigid surface. Test No.3 (Ning and Ghadiri, 1996) was conducted to check the effect of the restitution coefficient on the normal impact. Test No.4 (Renzo & Maio, 2004; Kharaz et al., 2001), Test No.5 (Maw et al., 1976; Wu et al., 2003) and Test No.6 (Vu-Quoc and Zhang, 1999a) were employed to check the oblique impact between a sphere and a rigid surface. Test No.7 and Test No.8 (Ooi and Chung, 2004) were conducted to check the oblique impact of two spheres. EDEM code was subjected to all of these benchmark tests and due to time constraint, PFC3D code was only checked against a subset of these tests. The corresponding input parameters are shown in Table 4.2. A multiplier for critical time step was set equal to 0.01 (1%) for all benchmark tests to ensure that the computational time step will have negligible effect on the numerical outcomes. The DEM results in these benchmark tests were compared with the analytical solutions described in the previous sections, experimental results and finite element results found in the literature.
4.4.1 Test No.1: Elastic normal contact of two identical spheres

First consider the elastic normal impact of two identical spheres with the same magnitude of velocity but in opposite directions, as shown in Figure 4.1. The input parameters are listed in Table 4.2. The incoming velocity is 10 m/s.

The normal contact force is plotted against the normal contact displacement in Figure 4.7. The DEM result shows that the unloading path of the force-displacement (FD) curve is practically the same as the loading path, indicating that there is no energy dissipation when the restitution coefficient is set to unity. As expected, the FD curve for DEM simulation using the Hertz-Mindlin contact model matches with the Hertz theory for elastic normal contact.
Table 4.1 Summary of benchmark test problems

<table>
<thead>
<tr>
<th>Case No.</th>
<th>Title</th>
<th>Objective</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Elastic normal contact of two identical spheres</td>
<td>Check the elastic normal contact between two spheres.</td>
<td>Timoshenko &amp; Goodier (1970)</td>
</tr>
<tr>
<td>2</td>
<td>Elastic normal contact of a sphere with a rigid surface</td>
<td>Check the elastic normal contact between a sphere and a surface.</td>
<td>Timoshenko &amp; Goodier (1970)</td>
</tr>
<tr>
<td>3</td>
<td>Normal contact for different restitution coefficients</td>
<td>Check the effect of damping ratio.</td>
<td>Ning &amp; Ghadiri (1996)</td>
</tr>
<tr>
<td>4</td>
<td>Oblique impact with a constant resultant velocity but different</td>
<td>Check the tangential force calculation between a sphere and a surface.</td>
<td>Renzo &amp; Maio (2004), Kharaz et al. (2001)</td>
</tr>
<tr>
<td></td>
<td>incident angles</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>Oblique impact with a constant normal velocity but different</td>
<td>Check the tangential force calculation between a sphere and a surface.</td>
<td>Maw et al. (1976), Wu et al. (2003)</td>
</tr>
<tr>
<td></td>
<td>tangential velocities</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>Oblique impact with a constant normal velocity but different</td>
<td>Check the tangential force calculation between a sphere and a surface.</td>
<td>Vu-Quoc &amp; Zhang (1999a)</td>
</tr>
<tr>
<td></td>
<td>angular velocities</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>Oblique impact of two identical spheres with a constant normal</td>
<td>Check the tangential force calculation between two spheres.</td>
<td>Designed by Ooi &amp; Chung (2004)</td>
</tr>
<tr>
<td></td>
<td>velocity and varying angular velocities</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>Oblique impact of two differently sized spheres with a constant</td>
<td>Check the tangential force calculation between two spheres.</td>
<td>Designed by Ooi &amp; Chung (2004)</td>
</tr>
<tr>
<td></td>
<td>normal velocity and varying angular velocities</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 4.2 DEM input parameters for benchmark tests

<table>
<thead>
<tr>
<th>Input parameters</th>
<th>Test No.1</th>
<th>Test No.2</th>
<th>Test No.3</th>
<th>Test No.4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young's modulus (N/m²)</td>
<td>4.800E+10</td>
<td>7.000E+10</td>
<td>3.800E+11</td>
<td>3.800E+11</td>
</tr>
<tr>
<td>Poisson ratio</td>
<td>0.20</td>
<td>0.30</td>
<td>0.23</td>
<td>0.23</td>
</tr>
<tr>
<td>Shear modulus (N/m²)</td>
<td>2.000E+10</td>
<td>2.692E+10</td>
<td>1.545E+11</td>
<td>1.545E+11</td>
</tr>
<tr>
<td>Friction coefficient</td>
<td>0.350</td>
<td>0.000</td>
<td>0.092</td>
<td>0.092</td>
</tr>
<tr>
<td>Restitution coefficient</td>
<td>1.000</td>
<td>1.000</td>
<td>different values</td>
<td>0.980</td>
</tr>
<tr>
<td>Density (Kg/m³)</td>
<td>2800</td>
<td>2699</td>
<td>4000</td>
<td>4000</td>
</tr>
<tr>
<td>Radius (m)</td>
<td>0.010</td>
<td>0.100</td>
<td>0.0025</td>
<td>0.0025</td>
</tr>
<tr>
<td>Velocity (m/s)</td>
<td>10</td>
<td>0.2</td>
<td>3.9</td>
<td>3.9</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Input parameters</th>
<th>Test No.5</th>
<th>Test No.6</th>
<th>Test No.7</th>
<th>Test No.8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young's modulus (N/m²)</td>
<td>2.08E+11</td>
<td>7.000E+10</td>
<td>7.000E+10</td>
<td>7.000E+10</td>
</tr>
<tr>
<td>Poisson ratio</td>
<td>0.30</td>
<td>0.20</td>
<td>0.20</td>
<td>0.20</td>
</tr>
<tr>
<td>Shear modulus (N/m²)</td>
<td>8.000E+10</td>
<td>2.917E+10</td>
<td>2.917E+10</td>
<td>2.917E+10</td>
</tr>
<tr>
<td>Friction coefficient</td>
<td>0.300</td>
<td>0.400</td>
<td>0.400</td>
<td>0.400</td>
</tr>
<tr>
<td>Restitution coefficient</td>
<td>1.000</td>
<td>0.500</td>
<td>0.500</td>
<td>0.500</td>
</tr>
<tr>
<td>Density (Kg/m³)</td>
<td>7850</td>
<td>2800</td>
<td>2800</td>
<td>2800</td>
</tr>
<tr>
<td>Radius (m)</td>
<td>1.00E-05</td>
<td>0.100</td>
<td>0.100</td>
<td>0.100</td>
</tr>
<tr>
<td>Normal velocity (m/s)</td>
<td>5</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
</tr>
</tbody>
</table>

Figure 4.8 shows the evolution of the normal contact force against time and the shape of the force-time curve is symmetric for this elastic normal contact. The contact duration, maximum normal contact displacement and contact force between the DEM result and analytical solutions obtained from Eqs. (4.2-4.4) respectively were compared in Table 4.3. The differences are less than 0.2 %.

Table 4.3 Comparison between DEM result and analytical solutions for elastic normal impact of two identical spheres

<table>
<thead>
<tr>
<th>Physical quantities</th>
<th>DEM result</th>
<th>Analytical solution</th>
<th>Difference (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Contact duration (µs)</td>
<td>40.341</td>
<td>40.295</td>
<td>0.12</td>
</tr>
<tr>
<td>Maximum displacement (µm)</td>
<td>274.000</td>
<td>274.113</td>
<td>0.04</td>
</tr>
<tr>
<td>Maximum force (N)</td>
<td>10712</td>
<td>10697</td>
<td>0.14</td>
</tr>
</tbody>
</table>
Figure 4.7 Force-displacement curve for elastic normal impact of two identical spheres

Figure 4.8 Force-time curve for elastic normal impact of two identical spheres
4.4.2 Test No.2: Elastic normal contact of a sphere with a rigid surface

Consider the elastic normal impact between a sphere and a rigid surface, as shown in Figure 4.2. The input parameters are listed in Table 4.2. The incoming velocity is 0.2 m/s.

Figure 4.9 depicts the plot of normal contact force versus normal contact displacement for the elastic collision. The DEM result shows no energy dissipation from the loading and unloading paths during the collision. The force displacement curves obtained from Hertz theory and from Zhang & Vu-Quoc’s finite element analysis (2002) are also plotted and they match with the DEM results. The plot of the normal contact force against time is shown in Figure 4.10. Table 4.4 presents the comparison for the contact duration, maximum normal contact displacement and contact force between the DEM result and analytical solutions obtained from Eqs. (4.5-4.7). It can be seen that the differences are very small at less than 0.6%.

<table>
<thead>
<tr>
<th>Physical quantities</th>
<th>DEM result</th>
<th>Analytical solution</th>
<th>Difference (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Contact duration (μs)</td>
<td>731.450</td>
<td>730.842</td>
<td>0.08</td>
</tr>
<tr>
<td>Maximum displacement (μm)</td>
<td>50.000</td>
<td>49.717</td>
<td>0.57</td>
</tr>
<tr>
<td>Maximum force (N)</td>
<td>11377</td>
<td>11370</td>
<td>0.06</td>
</tr>
</tbody>
</table>
Figure 4.9 Force-displacement curve for elastic normal impact of a sphere with a rigid plane

Figure 4.10 Force-time curve for elastic normal impact of a sphere with a rigid plane
4.4.3 Test No.3: Normal contact for different restitution coefficients

This test is to validate the case where a sphere normally impacts a rigid surface with different restitution coefficients (or different damping ratios). The input parameters are listed in Table 4.2 and the incoming velocity is 3.9 m/s. The input values for the restitution coefficient were set to be 0.0, 0.2, 0.4, 0.6, 0.8 and 1.0. Figure 4.11 illustrates the comparison of the ratio of rebound velocity to impact velocity obtained by computer simulation with the input value of the restitution coefficient. There is an exact agreement between the two, thus providing the verification that the DEM codes are correct in this respect.

![Figure 4.11 Comparison between computer simulated velocity ratio and the input value of the restitution coefficient](image)

Figure 4.11 Comparison between computer simulated velocity ratio and the input value of the restitution coefficient
4.4.4 Test No.4: Oblique impact with a constant resultant velocity but different incident angles

This test is to validate the case where a sphere impacts a rigid surface with a constant resultant velocity but different incident angles, as shown in Figure 4.12. The input parameters are listed in Table 4.2 and the constant resultant velocity is 3.9 m/s. The incident angle was varied between 5° and 85°.

![Figure 4.12](image)

Knowing that \( V_{cn} = -V_n = -V \cos(\theta) \) and \( V_{ct} = V_{st} = V_t = V \sin(\theta) \), Eqs. (4.35) and (4.40) can be rearranged as

\[
e_t = 1 - \mu(1 + e_s)\cot(\theta) \quad \text{for sliding regime} \tag{4.42}
\]

\[
e_t > 1 - \mu(1 + e_s)\cot(\theta) \quad \text{for sticking regime} \tag{4.43}
\]

Combining Eqs. (4.29), (4.31), (4.34) and (4.36) and knowing that \( \omega_1 = \omega_2 = \omega'_2 = 0 \), the post-collision angular velocity in the sliding regime can be expressed as

\[
\omega'_1 = -2.5 \frac{\mu(1 + e_s) V \cos(\theta)}{r_1} \tag{4.44}
\]
In Eq. (4.44), the minus sign indicates that the sphere spins clockwise after impact. From Eq. (4.38), the recoil angle on the contact path $\varphi$ can be related to the incident angle $\theta$ in the sliding regime as

$$\varphi = \tan^{-1} \left[ \frac{1}{\frac{e_n}{\tan(\theta) - 3.5\mu(1 + \frac{1}{e_n})}} \right]$$

(4.45)

The DEM results were compared with data obtained in equivalent experiments (Kharaz et al, 2001) and the analytical solutions from the previous section. Figure 4.13 shows the tangential coefficient of restitution based on the centre of mass $e$, against the angle of incidence $\theta$. The DEM result matches the analytical solutions: Eq. (4.42) in the sliding regime and Eq. (4.43) in the sticking regime. The plot also shows good agreement with the experimental result except for incident angle less than 10°. Impact for incident angle greater than a critical value $\theta_{critical}$ is seen to occur in sliding condition. Maw et al (1976) calculated this critical value to be approximately 28° when the restitution coefficient is unity. The DEM result gives a value of 30° which is close to Maw et al’s solution: the small difference is due to a value of 0.98 for the restitution coefficient in both the DEM simulation and the experiment.

The post-collision angular velocity $\omega'$ is plotted for various incident angles $\theta$, as shown in Figure 4.14. The DEM result follows the theoretical prediction given by Eq. (4.44) in the sliding regime and produces excellent agreement with observations in the experiment in both sliding and sticking regimes. A further indication is given in Figure 4.15, which shows the recoil angle against the incident angle. The DEM result follows the theoretical solution of Eq. (4.45) in the sliding regime and gives excellent match with the experimental data.
Figure 4.13 Simulated, theoretical and experimental tangential restitution coefficient $e_t$ versus incident angle $\theta$.

Figure 4.14 Simulated, theoretical and experimental post-collision angular velocity $\omega'$ versus incident angle $\theta$. 
Figure 4.15 Simulated, theoretical and experimental rebound angles $\phi$ versus incident angle $\theta$

4.4.5 Test No.5: Oblique impact with a constant normal velocity but different tangential velocities

This test is to validate the case where a sphere impacts a rigid surface with a constant normal velocity but at different tangential velocities, as shown in Figure 4.16. Consider an elastic oblique impact ($e_n = 1$) with friction as the only source of energy dissipation. The input parameters are listed in Table 4.2 and the constant normal velocity is 5 m/s. The tangential velocity is varied between 0.1 and 70.0 m/s.
Figure 4.16 A sphere impacting a rigid surface with a constant normal velocity and varying tangential velocities

Giving that $V_{cn} = -V_n$, $V_{st} = V_t$ and $e_n = 1$, Eq. (4.38) can be rewritten in a normalized form as

$$\frac{V'_t}{\mu V'_n} = \frac{V_t}{\mu V_n} - 7 \quad (4.46)$$

Similarly, Eq. (4.44) can be rearranged in a normalized form as

$$\frac{r_i \omega'_i}{\mu V_n} = -5 \quad (4.47)$$

In Eq. (4.47), the minus sign indicates that the sphere rotates clockwise after impact.

The DEM results were compared with the results obtained by Maw et al. (1976), finite element analysis results obtained by Wu et al. (2003) and the analytical solutions from Eqs. (4.46-4.47). Maw et al. presented an analytical solution for an oblique impact of a homogeneous elastic sphere on a half-space. Their calculation was based on Hertz theory (1896) for normal contact and Mindlin and Deresiewicz theory (1953) for tangential elastic frictional contact. The Poisson’s ratio of the material in Maw et al.’s calculation was 0.3, as adopted in the DEM simulation. Wu et al. conducted finite element analysis of an elastic oblique impact and the material properties in their calculation are the same as those in the DEM simulation except
that the sphere was rigid and the substrate was elastic in their computation whereas
the sphere can locally deform (overlap) in the contact region and the wall is rigid in
the DEM computation. Figure 4.17 depicts the variation of the normalized recoil
angle of the contact $\frac{V'}{\mu V'_n}$ with the normalized incident angle $\frac{V}{\mu V_n}$. It can be seen
that the DEM result agrees well in the sliding regime with all three solutions: Maw et
al.’s, Wu et al.’s FEA and the analytical solution given by Eq. (4.46). However, the
DEM result shows some discrepancy in the sticking regime with the solutions from
Maw et al. and Wu et al., with the DEM predicting smaller ratio of $\frac{V'}{\mu V'_n}$. This is
probably because the contact force model adopted in the DEM simulation is the
widely used Hertz-Mindlin no-slip simplified model and not the complete theory of
Hertz and Mindlin-Deresiewicz, as used in Maw et al.’s calculation. The normalized
post-collision angular velocity is plotted against the normalized incident angle in
Figure 4.18. The same observations can be made, with DEM giving an excellent
agreement in the sliding regime with FEA and analytical solution given by Eq.
(4.47), but producing some discrepancy in the sticking regime due to the Hertz-
Mindlin no-slip model employed in the DEM simulation. This discrepancy between
the DEM and FEA results in the sticking regime can be solved by using a more
complete Hertz-Mindlin contact force model (Thornton et al., 2001; Renzo and
Maio, 2004).
Figure 4.17 Normalized recoil angle versus normalized incident angle for varying initial tangential velocities

Figure 4.18 Normalized post-collision angular velocity versus normalized incident angle for varying initial tangential velocities
4.4.6 Test No.6: Oblique impact with a constant normal velocity but different angular velocities

This test is to validate the case where a sphere impacts a rigid surface with a constant normal velocity but different angular velocities, as shown in Figure 4.19. The input parameters are listed in Table 4.2 and the constant normal velocity is 0.2 m/s. The angular velocity was varied between 0.175 and 22.860 rad/s.

\[
V_n = \text{constant} \\
\omega = \text{varied}
\]

**Figure 4.19** A sphere impacting a rigid surface with a constant normal velocity and varying angular velocities

Knowing that \( V_{cn} = -V_n \) and \( V_{sf} = r_i \omega_i = V_s \), Eqs. (4.36) and (4.41) can be rearranged as

\[
\beta = -1 + 3.5\mu(1 + e_n)\frac{V_n}{V_s} \quad \text{for sliding regime} \tag{4.48}
\]

\[
\beta < -1 + 3.5\mu(1 + e_n)\frac{V_n}{V_s} \quad \text{for sticking regime} \tag{4.49}
\]

Similarly, Eq. (4.38) can be rearranged as

\[
\frac{V_s'}{V_n'} = \frac{7}{2\mu(1 + \frac{1}{e_n}) + \frac{1}{e_n} \frac{V_s}{V_n}} \tag{4.50}
\]

Figure 4.20 shows the DEM result for the variation of the tangential restitution coefficient based on the contact patch \( \beta \) with the quantity \( 3.5\mu(1 + e_n)\frac{V_n}{V_s} \) and
Figure 4.21 depicts the variation of the tangent of recoil angle on the contact patch $\frac{V'_x}{V'_n}$ with the tangent of incident angle $\frac{V_x}{V_n}$. It can be seen that for sliding collision, the tangential coefficient of restitution $\beta$ is a linear function of $\frac{V_n}{V_s}$ and that the tangent of the recoil angle $\frac{V'_x}{V'_n}$ is also a linear function of the tangent of the corresponding incident angle $\frac{V_x}{V_n}$. These relationships are as predicted theoretically by Eqs. (4.48) and (4.50). The above results also agree with the inequality Eq. (4.49). Figure 4.20 also shows that there are two important parameters that control the collision regimes: the larger the friction coefficient $\mu$ and the ratio $\frac{V_n}{V_s}$, the more likely that the collision is sticking.
Figure 4.20 Simulated and theoretical tangential restitution coefficient $\beta$ versus the quantity $3.5\mu(1 + e_n)V_n/V_s$.

Figure 4.21 Simulated and theoretical tangent of recoil angle $\frac{V_i}{V_n}$ versus tangent of incident angle $\frac{V_i}{V_n}$.
4.4.7 Test No.7: Oblique impact of two identical spheres with a constant normal velocity and varying angular velocities

This test is to validate the case where two identical spheres collide with a constant normal velocity but at different angular velocities. The normal and angular velocities of the two spheres are opposite as shown in Figure 4.22. The input parameters are listed in Table 4.2 and the constant normal velocity is 0.2 m/s. The angular velocity was varied between 0.175 and 22.860 rad/s.

![Diagram showing two identical spheres with constant normal velocity and varying angular velocities](image)

**Figure 4.22** Two identical spheres colliding with a constant normal velocity and varying angular velocities

Since the relative pre-collision tangential velocity on the contact path is zero, no tangential force is generated during this normal impact, i.e. $f_t = 0$ and $F_t = 0$. From Eqs. (4.11) and (4.14), we can deduce

$$V_{\alpha,1}' = V_{\alpha,2}' = 0$$  \hspace{1cm} (4.51)

Similarly, from Eqs. (4.13) and (4.16), we can deduce

$$\omega_1' = \omega_1, \quad \omega_2' = \omega_2$$  \hspace{1cm} (4.52)

Figure 4.23 shows the post-collision tangential velocity for Sphere 1 or Sphere 2 at the centre of mass for various pre-collision angular velocities. The DEM result shows that the post-collision tangential velocity for Sphere 1 or Sphere 2 at the
centre of mass is zero, which exactly matches the analytical solution given by Eq. (4.51). The post-collision angular velocities for Sphere 1 or Sphere 2 are plotted against pre-collision angular velocities in Figure 4.24, showing that DEM follows exactly the analytical prediction given by Eq. (4.52).

Figure 4.23 Post-collision tangential velocity at the centre of mass versus pre-collision angular velocity
Figure 4.24 Post-collision angular velocity versus pre-collision angular velocity

4.4.8 Test No.8: Oblique impact of two differently sized spheres with a constant normal velocity and varying angular velocities

This test is to validate the case where a small sphere with a constant normal velocity but different angular velocities collides with a big sphere which is stationary before collision, as shown in Figure 4.25. The density of the big sphere is 1000 times that for the small sphere and the radius of the big sphere is 5 times that for the small sphere. The input parameters for the small sphere are listed in Table 4.2. The constant normal velocity is 0.2 m/s. The angular velocity was varied between 0.175 and 22.860 rad/s. Considering the following two situations: a) the shear modulus of the big sphere is 1000 times that for the small sphere; and b) the big sphere has the same mechanical properties as the small sphere.
The DEM results for cases (a) and (b) were compared to the analytical solutions given by Eqs. (4.48) and (4.50). The case (Test No.6, in Section 4.4.6) where a sphere impacts a rigid surface with a constant normal velocity but different angular velocities (see Figure 4.19), using the same input parameters as those for the small sphere, is also shown for comparison. Figure 4.26 shows the variation of the tangential restitution coefficient based on the contact patch $\beta$ with the quantity $[3.5\mu(1+e_s)\frac{V}{V_t}]$. The variation of the tangent of recoil angle on the contact patch is plotted against the tangent of incident angle in Figure 4.27. It can be seen from both figures that the DEM results for case (a) and the case of Test No.6 match very well. This must be true and the reason is that since the big sphere has a mass of 125000 times and a shear modulus of 1000 times those for the small sphere, the big sphere serves as a rigid wall, which is equivalent to the case of Test No.6. For case (b) where the big sphere has the same mechanical properties as the small sphere, it produces an exact agreement in the sliding regime with those from the case (a), the case of Test No.6 and analytical solution, as theoretically predicted by Eqs. (4.48) and (4.50).
Figure 4.26 Simulated and theoretical tangential restitution coefficient $\beta$ versus quantity $[3.5\mu (1 + e) \frac{V_n}{V_s}]$

Figure 4.27 Simulated and theoretical tangent of recoil angle $\frac{V_s'}{V_n'}$ versus tangent of incident angle $\frac{V_s}{V_n}$
4.5 Summary

The analytical solutions obtained from elasticity for elastic normal impact between two spheres or a sphere with a rigid surface and the analytical solutions obtained from dynamics principles for oblique impact have been reviewed in this chapter. A set of benchmark tests were performed to validate the DEM codes and to enhance the understanding of fundamental impact phenomena. The DEM results in these benchmark tests were compared with the analytical solutions and the experimental or finite element results found in the literature.

All benchmark tests showed good to excellent match, providing a quantitative validation for the DEM codes. This gives confidence in the results of the large number of DEM simulations of the physical experiments in the study. The analytical solutions provide an excellent insight into particle impact mechanics and guidance on the suitability of the method for modelling various particle scale phenomena. The DEM results also provide further information on some aspects in the sticking regime for oblique impact, where the analytical solutions can only provide an upper bound.
Chapter 5

Measurement of DEM input parameters

5.1 Introduction

The input parameters used in DEM simulations were often simply given without any explanation as to where they came from, and seldom measured in laboratory tests, so the influence of the input parameters on the prediction outcomes can be rather obscure. In order to acquire meaningful results, it is essential that the parameters involved in the model are either carefully determined, or the effect of assuming certain values for these parameters is carefully explored. These parameters include the physical properties (mass, density and geometric shape parameters) and mechanical properties (Young’s modulus, Poisson’s ratio, friction coefficient, coefficient of restitution) of the grains. In this study, the majority of the parameters were determined experimentally using different laboratory tests.

The methodologies and apparatuses for measuring the main particle parameters (Young’s modulus, friction coefficient and restitution coefficient) for DEM models were devised. In this study, physical properties and mechanical properties of grains were measured for six types of corn grains (Figure 5.1 a) provided by a company and labelled CornA, CornB, CornC, CornD, CornE and CornF respectively, wheat grains (Figure 5.1 b) from Edinburgh, glass beads (Figure 5.1 c) from Sigmund Lindner and the large corn grains from Garst Seed (Figure 5.1 d). The measurements are all
described in Sections 5.2 and 5.3 below. Only the measured properties for glass beads and Garst corn grains were used in DEM simulations of several calibration experiments. The measurements made on the other types of wheat and corn grains are also presented in this chapter as they represent useful data that can be used for future DEM simulations or other purposes.

![Image of different grain samples](image_url)

**Figure 5.1** Different grain samples
5.2 Measurement of physical properties of grains

A sample of individual grains was weighed to determine the mean and coefficient of variation of the mass of single grains. For each type of corn grains from the company, 10 grains were selected randomly. For Garst corn and wheat, 30 grains were selected randomly. The scales can read to 0.0001g. The mean and coefficient of variation (CoV) are given in Table 5.1. Detailed measurements can be found in Appendix A (Table A.1, A.8 and A.9).

<table>
<thead>
<tr>
<th>Grain type</th>
<th>ComA</th>
<th>CornB</th>
<th>CornC</th>
<th>CornD</th>
<th>CornE</th>
<th>CornF</th>
<th>Garst corn</th>
<th>Wheat</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean value (g)</td>
<td>0.3516</td>
<td>0.2241</td>
<td>0.3281</td>
<td>0.3619</td>
<td>0.2012</td>
<td>0.3028</td>
<td>0.4273</td>
<td>0.0462</td>
</tr>
<tr>
<td>CoV (%)</td>
<td>4.6</td>
<td>11.3</td>
<td>19.8</td>
<td>11.1</td>
<td>13.2</td>
<td>8.7</td>
<td>6.3</td>
<td>21.7</td>
</tr>
</tbody>
</table>

The shape of the corn grains is generally irregular. A significant number of shape parameters may be required to describe them accurately. Practical measurements show that the various shapes may broadly be characterized by specifying selected orthogonal axes. For example, corn grains can be characterized by their length, width and thickness. The linear dimensions of grains were measured directly using digital callipers with an accuracy of 0.01 mm. The test results are listed in Table 5.2. Detailed measurements can be found in Appendix A (Table A.2-A.9).

<table>
<thead>
<tr>
<th>Grain type</th>
<th>ComA</th>
<th>CornB</th>
<th>CornC</th>
<th>CornD</th>
<th>CornE</th>
<th>CornF</th>
<th>Garst corn</th>
<th>Wheat</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean length (mm)</td>
<td>12.18</td>
<td>8.91</td>
<td>10.07</td>
<td>9.91</td>
<td>10.09</td>
<td>11.53</td>
<td>10.11</td>
<td>6.61</td>
</tr>
<tr>
<td>CoV (%)</td>
<td>5.9</td>
<td>8.2</td>
<td>9.0</td>
<td>8.7</td>
<td>7.3</td>
<td>6.5</td>
<td>8.2</td>
<td>6.3</td>
</tr>
<tr>
<td>Mean width (mm)</td>
<td>8.90</td>
<td>6.99</td>
<td>7.59</td>
<td>8.84</td>
<td>7.11</td>
<td>7.82</td>
<td>9.11</td>
<td>3.32</td>
</tr>
<tr>
<td>CoV (%)</td>
<td>4.0</td>
<td>8.1</td>
<td>8.6</td>
<td>12.5</td>
<td>7.7</td>
<td>4.0</td>
<td>4.9</td>
<td>10.4</td>
</tr>
<tr>
<td>Mean height (mm)</td>
<td>4.66</td>
<td>6.26</td>
<td>6.60</td>
<td>6.63</td>
<td>5.14</td>
<td>5.12</td>
<td>6.69</td>
<td>2.94</td>
</tr>
<tr>
<td>CoV (%)</td>
<td>9.6</td>
<td>6.3</td>
<td>9.0</td>
<td>13.9</td>
<td>14.4</td>
<td>14.6</td>
<td>16.5</td>
<td>9.2</td>
</tr>
</tbody>
</table>

In the measurement of the specific weight, three random samples for each type of corn grains from the company were also prepared and each sample consisted of 20 corn grains. The mass of each sample was measured as described above. The volume of each sample was measured by the water displacement method using a
measuring cylinder. The specific weight was calculated according to the mass and volume of corn grains. For Garst corn and Edinburgh wheat, each sample consisted of 10 and 50 grains respectively. The test results are shown in Table 5.3. Detailed measurements can be found in Appendix A (Table A.10, A.13 and A.16).

### Table 5.3 Specific weights for different type grains

<table>
<thead>
<tr>
<th>Grain type</th>
<th>ComA</th>
<th>ComB</th>
<th>CornC</th>
<th>CornD</th>
<th>CornE</th>
<th>CornF</th>
<th>Garst corn</th>
<th>Wheat</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean value (N/m³)</td>
<td>13000</td>
<td>12800</td>
<td>12300</td>
<td>12800</td>
<td>12900</td>
<td>12600</td>
<td>12600</td>
<td>12600</td>
</tr>
<tr>
<td>CoV (%)</td>
<td>1.4</td>
<td>6.1</td>
<td>0.2</td>
<td>0.9</td>
<td>4.3</td>
<td>1.8</td>
<td>1.1</td>
<td>1.8</td>
</tr>
</tbody>
</table>

Whilst bulk density is not a particle parameter, it is an important bulk property that depends on packing structure. The container used in the density tests has a volume of 1000 cm³, as shown in Figure 5.2. The “loose” bulk density was obtained by pouring the material through a funnel (with an outlet diameter of 20 mm) from a fixed small height. The “dense” bulk density was obtained by filling the cylinder and then shaken for 15 minutes using a sieve shaker as shown in Figure 5.2. No damage to the grains was observed during this process. The mould was topped up with grains and shaken until the mould was full. Three samples for each type of corn grains from the company and four samples for wheat were prepared respectively. Porosity in the loose and dense conditions can be determined from the specific weight and bulk density. The test results are shown in Tables 5.4 and 5.5. Detailed measurements can be found in Appendix (Table A.11, A.12, A.14 and A.15).

### Table 5.4 Loose bulk densities and void ratios for different type grains

<table>
<thead>
<tr>
<th>Grain type</th>
<th>CornA</th>
<th>CornB</th>
<th>CornC</th>
<th>CornD</th>
<th>CornE</th>
<th>CornF</th>
<th>Wheat</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean value (kg/m³)</td>
<td>850</td>
<td>810</td>
<td>800</td>
<td>850</td>
<td>820</td>
<td>830</td>
<td>720</td>
</tr>
<tr>
<td>CoV (%)</td>
<td>0.2</td>
<td>0.3</td>
<td>0.5</td>
<td>0.8</td>
<td>0.6</td>
<td>0.3</td>
<td>0.6</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.36</td>
<td>0.38</td>
<td>0.37</td>
<td>0.35</td>
<td>0.38</td>
<td>0.35</td>
<td>0.44</td>
</tr>
</tbody>
</table>

### Table 5.5 Dense bulk densities and void ratios for different type grains

<table>
<thead>
<tr>
<th>Grain type</th>
<th>CornA</th>
<th>CornB</th>
<th>CornC</th>
<th>CornD</th>
<th>CornE</th>
<th>CornF</th>
<th>Wheat</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean value (kg/m³)</td>
<td>880</td>
<td>850</td>
<td>810</td>
<td>870</td>
<td>840</td>
<td>860</td>
<td>790</td>
</tr>
<tr>
<td>CoV (%)</td>
<td>0.7</td>
<td>0.7</td>
<td>0.5</td>
<td>0.3</td>
<td>0.9</td>
<td>0.3</td>
<td>0.4</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.34</td>
<td>0.35</td>
<td>0.35</td>
<td>0.34</td>
<td>0.36</td>
<td>0.33</td>
<td>0.38</td>
</tr>
</tbody>
</table>
It can be seen from Table 5.2 that the variation coefficients (ratio of standard deviation to mean) regarding length, width, and height for CornA, CornB, and CornC are less than 10%, whilst the variation coefficients for CornD, CornE, CornF, Garst corn and wheat are less than 17%.

The range of the bulk density for corn and wheat grains in the silo design book (Rotter, 2001) is 7.0-8.5 KN/m$^3$ (720-870 kg/m$^3$) and 7.5-9.0 KN/m$^3$ (760-920 kg/m$^3$), respectively. Moya et al. (2002) presented the bulk density for corn grains at different normal pressures. These values range from 745 to 767 kg/m$^3$ as the normal pressures vary from 0 to 150 kPa. Table 5.4 shows that the mean values for the loose bulk density for the six grain types range from 800 to 850 kg/m$^3$, whilst the mean values for the dense bulk density range from 810 to 880 kg/m$^3$ in Table 5.5. The values for wheat grains arrange from 720 to 790 kg/m$^3$. It can be seen that these values are close to those in the literature.
5.3 Measurement of mechanical properties of grains

5.3.1 Measurement of particle Young's modulus

In this study, the ASAE Standard single particle compression test using a spherical indenter (Figure 5.3) was initially used to determine the particle stiffness required for DEM simulations. The spherical indenter may be used for corn grains with very flat surfaces, such as CornA and CornF (Codes for corn samples). However, it was observed that when the corn grains are not very flat, the indenter slips and bends during the test, as shown in Figure 5.4. In these cases, the contact area is no longer circular or elliptical and the line of the applied load is also no longer vertical. Consequently, the formula in the ASAE Standard would not be valid. Thus, the indenter method is not suitable for corn grains that do not have sufficiently flat surfaces, such as CornB, CornC, CornD and CornE. To overcome these, it is proposed that a vertical compression of the particle between two rigid platens is conducted. A 3D laser scanner (3D Scanners Ltd., 1998) was used to capture the three-dimensional surface geometry of individual grains. The scanned data were processed to more accurately measure the radii of curvature. This improved method for determining the Young's modulus for corn grains was developed by first reviewing a set of transcendental equations (Hertz, 1896) which Hertz derived for more general cases; secondly, providing a simplified approach to solve these equations. In addition, the effect of the assumed value for Poisson's ratio on the Young's modulus was examined. The two methods are described below.
Figure 5.3 ASAE method with a spherical indenter

Figure 5.4 The spherical indenter bent during the compression test
5.3.1.1 Theoretical considerations

(1) The ASAE Standard method:

According to the ASAE standard (1996), the spherical indenter was chosen to
determine the modulus of elasticity for corn grains. The formula is given by (Shelef
and Mohsenin, 1969)

\[ E = \frac{0.338K_c^{3/2} P(1-\nu^2)}{\alpha^{3/2}} \left( \frac{4}{d} \right)^{1/2} \]  

(5.1)

where \( E \) is the modulus of elasticity of a single corn grain; \( P \) is the load applied;
\( \alpha \) is the deformation of the grain; \( \nu \) is the Poisson’s ratio of the grain; \( d \) is the
diameter of the indenter and \( K_c \) is a geometric constant depending on the principal
radii of curvature of the contacting bodies. Eq. (5.1) is based on Hertzian contact
with the assumption that the radii of curvature of the corn grain are assumed to be
infinite, giving a value of \( K_c = 1.351 \). For an indenter with a diameter of 2 mm and
an assumed Poisson’s ratio of 0.4, Eq. (5.1) can be rewritten as

\[ E = \frac{0.63 \times P}{\alpha^{3/2}} \]  

(5.2)

Eq. (5.2) will be applied to the test results in Section 5.3.1.3 below.

(2) The proposed rigid platen compression method:

The more general Hertzian contact theory (Hertz, 1896; Kosma and Cunningham
1962; Timoshenko and Goodier, 1970) is briefly reviewed here to derive an
appropriate approach to interpret this test. Consider two bodies with different radii
in contact, as illustrated in Figure 5.5(a). \( R_1 \) and \( R'_1 \) denote the principal radii of
curvature at the point of contact of one of the bodies, and \( R_2 \) and \( R'_2 \) those of the
other, and \( H \) the angle between the normal planes containing the curvatures
$1/R_1$ and $1/R_2$. $E_1$ and $\nu_1$ are the Young's modulus and Poisson's ratio for the lower body, and $E_2$ and $\nu_2$ those for the upper body. If we press the bodies together by the load $P$ in the direction of the normal to the tangent plane at $O$, the surface of contact will have an elliptical boundary with the major and minor radii ($a$ and $b$ respectively), as shown in Figure 5.5(b).

Hertz made the following assumptions: (1) The contacting bodies are isotropic and Hooke's law holds; (2) The radii of curvature of the contacting bodies are large in comparison with the dimensions of the contact area; (3) The compressive stress distribution is proportional to the ordinates of a semi-ellipsoid constructed on the surface of contact; and (4) The contacting bodies are infinitely large, or the contact stresses vanish at the opposite end of the bodies. Based on the above assumptions, the solution for the major and minor radii ($a$ and $b$) in the contact ellipse and the normal deformation ($\alpha$) of the two contacting bodies together with a factor ($\varepsilon$) is implicitly given by the following equations.

$$ A = \frac{3P(k_1 + k_2)}{2a^3 \sin^2 \varepsilon} \left[ J(\sin^2 \varepsilon) - J(\sin^2 \varepsilon) \right] \tag{5.3} $$
\[ B = \frac{3P(k_1 + k_2)}{2a^3 \sin^2 \varepsilon} \left[ J(\sin^2 \varepsilon)/\cos^2 \varepsilon - I(\sin^2 \varepsilon) \right] \] (5.4)

\[ \alpha = \frac{3P(k_1 + k_2)}{2a} I(\sin^2 \varepsilon) \] (5.5)

\[ b = a \cos \varepsilon \] (5.6)

Where \( I(\sin^2 \varepsilon) \) and \( J(\sin^2 \varepsilon) \) are the complete first and second order elliptical integrals respectively, and are defined in Eqs. (5.7-5.8). \( A \) and \( B \) are constants depending on the magnitudes of the principal curvatures of the surface in contact and on the angle between the planes of principal curvatures of the two surfaces. The constants \( A \) and \( B \) can be expressed in Eqs. (5.9-5.10). \( k_1 \) and \( k_2 \) are constants related to the Young’s modulus and Poisson’s ratio, as written in Eq. (5.11).

\[ I(\sin^2 \varepsilon) = \int_0^{\pi/2} \frac{d\phi}{(1 - \sin^2 \phi \sin^2 \varepsilon)^{1/2}} \] (5.7)

\[ J(\sin^2 \varepsilon) = \int_0^{\pi/2} (1 - \sin^2 \phi \sin^2 \varepsilon)^{1/2} d\phi \] (5.8)

\[ A = \frac{1}{4} \left( \frac{1}{R_1} + \frac{1}{R_1'} + \frac{1}{R_2} + \frac{1}{R_2'} \right) \]

\[ -\frac{1}{4} \sqrt{\left[ \left( \frac{1}{R_1} - \frac{1}{R_1'} \right) + \left( \frac{1}{R_2} - \frac{1}{R_2'} \right) \right]^2 - 4\left( \frac{1}{R_1} - \frac{1}{R_1'} \right) \left( \frac{1}{R_2} - \frac{1}{R_2'} \right) \sin^2 H} \] (5.9)

\[ B = \frac{1}{4} \left( \frac{1}{R_1} + \frac{1}{R_1'} + \frac{1}{R_2} + \frac{1}{R_2'} \right) \]

\[ +\frac{1}{4} \sqrt{\left[ \left( \frac{1}{R_1} - \frac{1}{R_1'} \right) + \left( \frac{1}{R_2} - \frac{1}{R_2'} \right) \right]^2 - 4\left( \frac{1}{R_1} - \frac{1}{R_1'} \right) \left( \frac{1}{R_2} - \frac{1}{R_2'} \right) \sin^2 H} \] (5.10)
Although Hertz obtained the analytical solution, it is implicitly expressed and impractical to use. Accordingly, the analytical solution needs to be expressed explicitly for practical purpose. It may be seen that there are four equations Eqs. (5.3-5.6) and four unknowns \((a, b, \alpha \text{ and } \varepsilon)\). In this study, the following approach was developed to solve these four unknowns. Consider the dimensionless parameter \(\beta^*\), which is defined as

\[
\beta^* = \frac{B - A}{B + A}
\]  

Eq. (5.12) can be expressed as the following equation by substituting Eqs. (5.3-5.4) into Eq. (5.12).

\[
\beta^* = 1 - 2\left[I(\sin^2 \varepsilon) - J(\sin^2 \varepsilon)\right] \cot \varepsilon = J(\sin^2 \varepsilon)
\]  

Let \(y = \sin^2 \varepsilon\) and Eq. (5.13) can be rewritten as

\[
2[I(y) - J(y)](1 - y) = (1 - \beta^*) y J(y)
\]  

It can be seen that the above equation forms a non-linear equation. This equation can be solved using an appropriate iteration technique (for example, bisection or Newton-Raphson method) to determine \(y\). In the present study, a Fortran program was coded to obtain the solution using the bisection method. The Fortran program is listed in Appendix F. Using the example for CornD-3 \((R_1 = 3.0 \text{ mm}, R_1' = 2.4 \text{ mm})\), the solution to Eq. 5.14 was found to be \(y = 0.236\), as shown in Figure 5.6.
Figure 5.6 2[J(y)−J'(y)](1−y)−(1−β^*) y J(y) versus y in the example for ComD-3

Once $y$ is determined, the solution for $a$, $b$, $\alpha$ and $\epsilon$ can be explicitly expressed as follows:

$$a = \sqrt[3]{\frac{3P(k_1 + k_2)J(y)}{2(B + A)(1 - y)}}$$ \hspace{1cm} (5.15)

$$b = \sqrt{(1 - y)^3} \sqrt[3]{\frac{3P(k_1 + k_2)J(y)}{2(B + A)(1 - y)}}$$ \hspace{1cm} (5.16)

$$\alpha = \sqrt[3]{\frac{9(k_1 + k_2)^2 (B + A)(1 - y)I^3(y)P^2}{4J(y)}}$$ \hspace{1cm} (5.17)

$$\epsilon = \sin^{-1} \sqrt{y}$$ \hspace{1cm} (5.18)
Under testing conditions used in Section 5.3.1.2, \((R_2 \to \infty, R_1 \to \infty, k_2 = 0,\) and \(\nu_1 = 0.4\)), the Young’s modulus of single corn grain can then be expressed as

\[
E_i = \frac{1 - \nu_i^2}{\pi} \left[ \frac{9(R_1 + R_1')(1 - y)J^3(y)P^2}{8R_1R_1' \alpha^3 J(y)} \right]^{1/2}
\]  
(5.19)

Eq. (5.19) will be applied to the test results in Section 5.3.1.3 below. The following procedure can be used to determine the Young’s modulus for a single grain without solving the nonlinear equation (Eq. 5.14).

1. Determine the value of \(y\) from Figure 5.7 according to the ratio \((R_1'/R_1)\).

2. Determine the value of \(\left[ \frac{(1 - y)J^3P^2}{\alpha^3 J(y)} \right]^{1/2}\) from Figure 5.8 according to \(y\) and \(\alpha\) (normal contact displacement).

3. Calculate the Young’s modulus by using Eq. 5.19.
Figure 5.7 The solution $y$ versus $(R_1'/R_1)$

Figure 5.8 $\left(\frac{(1-y)P^2}{\alpha^3 J(y)}\right)^{1/2}$ versus $y$
5.3.1.2 Description of the experiments

All six types of corn grains (CornA, CornB, CornC, CornD, CornE and CornF) were tested. The compression tests were carried out using an Instron machine (Model 4500 Testing System), as described in Appendix B. The germ-side surface of each kernel was lightly sanded (in order that it is very flat and the deformation on this surface can be assumed to be negligible during the compression) and the kernels were glued, germ-side down, to a flat metal plate. The vertical load was applied to the surface of the kernel on the horny endosperm. Both testing methods, the ASAE Standard indenter method (Figure 5.3) and proposed method of compression between rigid platens (Figure 5.9), were performed.

In the ASAE Standard method, testing conditions were as follows:

1. Although ASAE specifies that the spherical indenter should have a radius of curvature of 0.838 mm. In practice, this dimension was very difficult to fabricate and could not be purchased even through suppliers recommended by ASAE. The closest indenter that could be sourced from the supplier has a radius of 1 mm and that was used instead.
2. The radii of curvature of corn kernels were assumed to be infinite.
3. The Poisson’s ratio of corn grains was assumed to be 0.4.
4. The Young's modulus was determined for applied load of 2.26 kg (22.2 N), as recommended in the ASAE Standard.

In the proposed rigid platen compression method, testing conditions were as follows:

1. The spherical indenter was replaced with a rigid cylinder, as described in Section 5.3.1.
2. The radii of curvature of corn kernels were measured using a 3D laser scanner (3D Scanners Ltd., 1998), as described in Appendix C.
3. The Poisson’s ratio of corn grains was assumed to be 0.4.
4. The Young’s modulus was determined for applied load of 2.26 kg (22.2 N).
5.3.1.3 Test results and discussions

The 3D laser scanner was used to capture the three-dimensional surface geometry of individual grains. Figures 5.10 and 5.11 show typical X-Z and Y-Z plane curves for a single grain (CornD), that intersect at the point of contact (the highest point). The radii of curvature in the mutually perpendicular planes can be determined from the scanned data and used to determine the Young’s modulus. Three representative points (the highest point and another two points, located at ±1 mm with respective to the highest point) were selected to determine the radius of curvature in the local contact region. The fitted curve was checked against the measured points to make sure that the fit is good. Using the example for CornD-3 (Figures 5.10 and 5.11), the values of the radii of curvature on the X-Z and Y-Z planes are 3.0 mm and 2.4 mm, respectively. For the chosen load of 22.2 N (ASAE reference value), the values of $a$ and $b$ can be calculated from Eqs 5.15-5.16 as 0.029 mm and 0.025 mm, respectively. The radii of curvature evaluated from the scanned geometry for the six kinds of corn grains can be found in Appendix A (Table A.18).
The Young's modulus for each corn type using the ASAE indenter method is shown in Table 5.6. Table 5.6 also gives the corresponding results from the proposed rigid platen compression method. Similarly, the Young’s modulus for glass beads is determined using the proposed rigid platen compression method and listed in Table 5.7. The Young’s modulus for wheat grains is listed in Table 5.7 as well and determined according to ASAE standard where some approximation for the radii of curvature of a typical wheat grain is made. Detailed measurements can be found in Appendix A (Table A.17-A.20).

### Table 5.6 Young’s moduli for six types of corn grains

<table>
<thead>
<tr>
<th>Corn type</th>
<th>Mean Young’s modulus (MPa) (based on the ASAE indenter method)</th>
<th>Mean Young’s modulus (MPa) (based on the proposed method)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CornA</td>
<td>900</td>
<td>1320</td>
</tr>
<tr>
<td>CornB</td>
<td>Not measurable</td>
<td>2320</td>
</tr>
<tr>
<td>CornC</td>
<td>Not measurable</td>
<td>1330</td>
</tr>
<tr>
<td>CornD</td>
<td>Not measurable</td>
<td>1770</td>
</tr>
<tr>
<td>CornE</td>
<td>Not measurable</td>
<td>2160</td>
</tr>
<tr>
<td>CornF</td>
<td>1040</td>
<td>1040</td>
</tr>
</tbody>
</table>

### Table 5.7 Young’s moduli for glass beads and wheat grains

<table>
<thead>
<tr>
<th>Grain type</th>
<th>Test method</th>
<th>Mean Young’s modulus (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Glass beads</td>
<td>based on the proposed method</td>
<td>40800</td>
</tr>
<tr>
<td>Wheat grains</td>
<td>based on the ASAE standard (parallel plate contact)</td>
<td>452</td>
</tr>
</tbody>
</table>

In general, the value of the Poisson’s ratio for any material ranges from 0.0 to 0.5. However, it is unlikely that the Poisson’s ratio for corn grains would take on a value less than that of steel (0.3) (Amold and Roberts, 1969). Accordingly, the practical range for corns can be narrowed to 0.3-0.5. Figure 5.12 shows the relationship between the evaluated Young’s modulus and the assumed Poisson’s ratio for CornB corn. The curves obtained for the remaining corn types are quite similar to the one shown here. The Poisson’s ratio was assumed to be 0.4 in the calculations presented so far, as per ASAE Standard. Figure 5.12 shows that the actual Young’s modulus should be lower if the Poisson’s ratio for the corn is larger than the assumed value of 0.4. For the range of the Poisson’s ratio between 0.3 and 0.5, the calculated Young’s modulus varies by some 21%.

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The range of the Young’s moduli for the six types of corn grains based on the proposed rigid platen compression method is 1040-2320 MPa with a mean of 1660 MPa and a coefficient of variation of 31%.

A reference value of the Young’s modulus for yellow dent hybrid corn (WF9MST×H71) (Oh43RF×B37RF) is given as 2030 MPa in the ASAE Standard (1996). This value is comparable with the measurements obtained in this study. The ASAE indenter method is here compared with the proposed compression method. The average Young’s moduli for CornA and CornF based on the ASAE method are 900 and 1040 MPa respectively, whilst those based on the proposed method are 1320 and 1040 MPa. The result obtained from the ASAE method thus matches that from the proposed method for CornF corn but differs significantly for CornA corn. The ASAE method is not suitable for corn grains such as CornB, CornC, CornD and CornE because they are not flat, thus causing the spherical indenter to slip and bend during the test.
Figure 5.10 Curve in X-Z plane (CornD corn)

Figure 5.11 Curve in Y-Z plane (CornD corn)
In the study by Shelef and Mohsenin (1969), the upper surface of kernels was finely sanded by means of a specially built mechanical sander to make the upper surface flat. The exposed area consisted of horny endosperm, varying in depth, and floury endosperm at the dent. However, this process may disturb the stiffness and strength of corn grains. In contrast, the upper surface of kernels was not tempered with in the proposed rigid platen compression method. The proposed method together with the 3D laser technique can be applied to any irregularly shaped corn grain, regardless of size and shape. In addition, the loading used appears to be very stable during the compression test.

**Figure 5.12** Effect of the Poisson’s ratio on Young’s modulus determination
5.3.2 Measurement of particle-surface friction coefficient

5.3.2.1 Theoretical considerations and description of the experiments

Figures 5.13 and 5.14 show the sliding friction apparatus and setup. Three corn grains are selected randomly. The germ-side surface of each kernel is sanded until all three have the same height. To make sure of this, they are put on a horizontal surface, the test plate is put on top of the three corn grains, and the level of the test plate can be checked using a spirit level. After this verification, three grains are then glued, horny endosperm-side up, on the horizontal base plate, as shown in Figure 5.13. The test plate is not glued but placed on top of the three grains and the level is checked again to ensure that it is horizontal. During the test, the inclination of the base plate is gradually increased using a jack, until relative sliding between the grains and the test plate occurs. The angle $\theta$ of the inclination of the base plate at this instant is calculated from the height measurement of the ruler (Figure 5.14). The static particle-surface friction coefficient ($\mu$) can be determined from Eq. (5.20)

$$\mu = \tan \theta$$

(5.20)

In the sliding friction apparatus, the ruler perpendicular to the bottom plate is located at a distance of 500 mm from the hinge and it can read to 0.5 mm. Accordingly, the measurement of the angle has an accuracy of approximately 0.06°.

5.3.2.2 Test results and discussions

The sliding friction tests were carried out on different material plates for all grain samples. Three different surfaces were tested: acrylic, steel and aluminium. Three samples for each type were tested. Each test was repeated three times for six types of corn grains from the company and five times for Garst corn grains, wheat grains and glass beads. Figure 5.15 shows the friction coefficients obtained for three samples of corn CornA on steel and aluminium. The data obtained for the remaining corn types are quite similar to the one shown here. The results for all grains on the aluminium
plate, stainless steel plate and acrylic plate are shown in Table 5.8. Detailed measurements can be found in Appendix A (Table A.21-A.25).

As shown in Table 5.8 (or Table A.21-A.25), the variation coefficient (ratio of standard deviation to mean) for each test is less than 10% and the variation coefficient for each type grain is also less than 12%. The sliding friction test is thus stable and reproducible.

The friction coefficients for the six corn types with the aluminium test plate vary from 0.226 to 0.276, whilst the corresponding range for the stainless steel test plate is 0.476-0.596. The friction coefficient is shown to be dominated by the roughness and type of the metal plate, and the different types of corn grains appear to have only small effect on the friction coefficient. It should also be noted that the higher friction coefficient measured for the stainless steel plate in this study might be due to the features of this particular test plate. The stainless steel test plate was obtained from a silo manufacturer.

Individual particle-particle friction can be measured for perfect spheres (e.g. O'Sullivan et al., 2004a), but no method is known for particles of other shapes, especially for irregularly shaped agricultural grains.
Figure 5.13 Sliding friction apparatus setup

Figure 5.14 Sliding friction apparatus
Figure 5.15 Friction coefficient measurements for Corn CornA

Table 5.8 Friction coefficients for different type grains

<table>
<thead>
<tr>
<th>Grain type</th>
<th>Plate material</th>
<th>Friction coefficient</th>
<th>CoV (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CornA</td>
<td>Aluminium</td>
<td>0.226</td>
<td>5.5</td>
</tr>
<tr>
<td>CornA</td>
<td>Stainless steel</td>
<td>0.519</td>
<td>5.2</td>
</tr>
<tr>
<td>CornB</td>
<td>Aluminium</td>
<td>0.249</td>
<td>8.5</td>
</tr>
<tr>
<td>CornB</td>
<td>Stainless steel</td>
<td>0.476</td>
<td>5.8</td>
</tr>
<tr>
<td>CornC</td>
<td>Aluminium</td>
<td>0.256</td>
<td>2.9</td>
</tr>
<tr>
<td>CornC</td>
<td>Stainless steel</td>
<td>0.569</td>
<td>4.8</td>
</tr>
<tr>
<td>CornD</td>
<td>Aluminium</td>
<td>0.276</td>
<td>9.9</td>
</tr>
<tr>
<td>CornD</td>
<td>Stainless steel</td>
<td>0.535</td>
<td>1.0</td>
</tr>
<tr>
<td>CornE</td>
<td>Aluminium</td>
<td>0.263</td>
<td>3.0</td>
</tr>
<tr>
<td>CornE</td>
<td>Stainless steel</td>
<td>0.596</td>
<td>4.4</td>
</tr>
<tr>
<td>CornF</td>
<td>Aluminium</td>
<td>0.254</td>
<td>5.6</td>
</tr>
<tr>
<td>CornF</td>
<td>Stainless steel</td>
<td>0.553</td>
<td>3.6</td>
</tr>
<tr>
<td>Garst corn</td>
<td>Acrylic</td>
<td>0.335</td>
<td>8.4</td>
</tr>
<tr>
<td>Wheat</td>
<td>Acrylic</td>
<td>0.212</td>
<td>11.6</td>
</tr>
<tr>
<td>Glass bead</td>
<td>Acrylic</td>
<td>0.244</td>
<td>6.4</td>
</tr>
</tbody>
</table>
5.3.3 Measurement of particle-surface restitution coefficient

The coefficient of restitution is not a material constant and depends on the geometry and materials as well as impact velocity (LoCurto, et al., 1997; Smith and Liu, 1992). However, due to the uncertainty in how the mechanism of particle-particle and particle-surface collisions is governed by the geometry, material properties and impact conditions, the coefficient of restitution is almost always considered to be a constant in DEM simulations. Experimental measurement of the coefficient of restitution in a certain range of impact velocities can be used to simulate granular flow.

5.3.3.1 Theoretical considerations

The three definitions for the coefficient of restitution are described as follows:

(1) Normal restitution coefficient $e_n$ and tangential restitution coefficient $e_t$ are given by (Sharma and Bilanski, 1971; Lorenz et al., 1997; Gorham and Kharaz, 2000; Kharaz et al., 2001; Chau et al., 2002)

$$e_n = \frac{V_{out,N}}{V_{in,N}} \quad \text{and} \quad e_t = \frac{V_{out,T}}{V_{in,T}}$$

(5.21)

where $V_{out,N}$ and $V_{in,N}$ are the magnitudes of the normal component of the rebounding and incoming velocities; $V_{out,T}$ and $V_{in,T}$ are the magnitudes of the tangential component of the rebounding and incoming velocities.

(2) Resultant restitution coefficient $e_R$ is given by (Yang and Schrock, 1994; Chau et al., 2002)

$$e_R = \frac{V_{out}}{V_{in}}$$

(5.22)

where $V_{out}$ and $V_{in}$ are the rebounding and incoming velocities, respectively.
(3) Energy restitution coefficient $e_e$ is given by (Johnson, 1985; LoCurto et al., 1997)

$$e_e = \left( \frac{E_{\text{out}}}{E_{\text{in}}} \right)^{1/2}$$  \hspace{1cm} (5.23)

where $E_{\text{out}}$ and $E_{\text{in}}$ are the kinetic energies after and before impact, respectively.

The energy restitution coefficient is a measure of the energy lost during a collision. When perfect spheres rebound vertically under normal impact, the normal, resultant and energy restitution coefficients will be identical since the horizontal velocity and angular velocity are zero. For impact involving particle rotation such as oblique impact of sphere or impact of non-spherical particle, ignoring particle rotation in the first two definitions (Eqs 5.21 and 5.22) will lead to inaccurate evaluation of the restitution coefficient. The energy coefficient of restitution is thus the most appropriate for non-spherical particles.

Let us consider an irregularly shaped particle falling freely from the height $H$, as illustrated in Figure 5.16 (a). It rebounds randomly and two orthogonal views of the rebounding trajectory of the particle, as shown in Figures 5.16 (b) and (c), are captured using a high-speed camera by means of an appropriately oriented mirror (Figure 5.18). Three consecutive pairs of position immediately after impact are selected in order to calculate the coefficient of restitution. The differences in the coordinates between position A and position C are denoted by $\Delta x$, $\Delta y$ and $\Delta z$, respectively. Similarly, the differences in the rotations are denoted by $\Delta \theta_x$, $\Delta \theta_y$ and $\Delta \theta_z$, respectively. Since the moment (taken about the mass centre of the particle) about the z direction, which is caused by the tangential force during the impact process, is expected to be much smaller than the moments in the x and y directions, $\Delta \theta_z$ may be ignored. By employing the central difference scheme, the linear and angular velocities at position B for a given time step $\Delta t$ can be expressed as follows:
\[ V_{\text{out},X} = \frac{\Delta x}{2\Delta t}, \quad V_{\text{out},Y} = \frac{\Delta y}{2\Delta t}, \quad V_{\text{out},Z} = \frac{\Delta z}{2\Delta t} \] 

(5.24)

\[ \omega_x = \frac{\Delta \theta_x}{2\Delta t}, \quad \omega_y = \frac{\Delta \theta_y}{2\Delta t}, \quad \omega_z = 0 \] 

(5.25)

where \( V_{\text{out},X}, V_{\text{out},Y} \) and \( V_{\text{out},Z} \) are the linear velocities in the x, y and z directions, respectively. \( \omega_x, \omega_y \) and \( \omega_z \) are the angular velocities in the x, y and z directions, respectively. It should be noted that the angular velocity in the z direction is assumed to be negligible.

![Figure 5.16 A schematic of the rebounding motion of an irregularly shaped particle](image)

The incoming velocity can be expressed as

\[ V_{\text{in}} = \sqrt{2gH} \] 

(5.26)

where \( H \) is the free drop height and \( g \) is the gravitational constant (i.e. 9.81 m/s²).

This equation can be verified from the analysis of images taken immediately before impact. From Eq. (5.24), the resultant velocity after impact can further be expressed as
From the definitions in Eqs. (5.21-5.22), the normal and resultant restitution coefficients can be rewritten as

\[
\begin{align*}
    e_n &= \frac{V_{out,N}}{V_{in,N}} = \frac{V_{out,z}}{\sqrt{2gH}} \\
    e_R &= \frac{V_{out}}{V_{in}} = \frac{\sqrt{V_{out,x}^2 + V_{out,y}^2 + V_{out,z}^2}}{\sqrt{2gH}}
\end{align*}
\tag{5.28-5.29}
\]

Now let us focus on the energy restitution coefficient. Based on the rigid body theory (Meriam and Kraige, 2003) and the fact that the angular velocity \( \omega \) is neglected, the kinetic energies before and after impact can be expressed as

\[
\begin{align*}
    E_{in} &= mgH \\
    E_{out} &= mgH_v + \frac{1}{2} mV_{out}^2 + \frac{1}{2} (I_{xx} \omega_x^2 + I_{yy} \omega_y^2 - 2I_{xy} \omega_x \omega_y)
\end{align*}
\tag{5.30-5.31}
\]

where \( H_v \) is the bounce height at position B and \( m \) is the mass of the particle. \( I_{xx} \) and \( I_{yy} \) are the mass moments of inertia about the x and y axes at the mass centre, while \( I_{xy} \) is the product of inertia about the x-y axes. If \( I_{xx}, I_{yy} \) and \( I_{xy} \) are given, then \( E_{out} \) and \( E_{in} \) can be calculated (\( \omega_x, \omega_y \) and \( V_{out} \) are calculated from Eqs. 5.25 and 5.27). The energy restitution coefficient can then be evaluated according to the definition in Eq. (5.23).

The remaining issue is to obtain \( I_{xx}, I_{yy} \) and \( I_{xy} \) corresponding to the orientation at position B. This information is obtained introducing the 3D laser scanning technique. The procedure for calculating \( I_{xx}, I_{yy} \) and \( I_{xy} \) is described below.
Consider an irregularly shaped particle in some orientation, as shown in Figure 5.17. The three-dimensional surface geometry of this particle is captured using the 3D laser scanner. The scanned data is processed and recorded by means of a solid modelling software. By using an appropriate numerical integration scheme, the mass moments and products of inertia in this orientation at the mass centre may be calculated as follows:

\[
I_{xx} = \int (\bar{y}^2 + \bar{z}^2) \, dm, \quad I_{yy} = \int (\bar{z}^2 + \bar{x}^2) \, dm, \quad I_{zz} = \int (\bar{x}^2 + \bar{y}^2) \, dm
\]

\[
I_{xy} = \int \bar{x} \bar{y} \, dm, \quad I_{yz} = \int \bar{y} \bar{z} \, dm, \quad I_{zx} = \int \bar{z} \bar{x} \, dm
\]

where the symbols have the same meaning as previously stated, but refer to the system of local Cartesian coordinates \( \bar{x} \), \( \bar{y} \) and \( \bar{z} \) (Figure 5.17). Using the same solid modelling software to match the images from the high-speed camera, the orientation at position B may be determined. Accordingly, the transformation matrix \([T]\) can be calculated as

\[
[T] = \begin{bmatrix}
T_{11} & T_{12} & T_{13} \\
T_{21} & T_{22} & T_{23} \\
T_{31} & T_{32} & T_{33}
\end{bmatrix}
\]

where the direction cosines of the x axis are \( T_{11} \), \( T_{21} \) and \( T_{31} \) in the Cartesian coordinates \( \bar{x} \), \( \bar{y} \) and \( \bar{z} \). Similar notations also apply to the y and z axes. The inertia matrix at position B can be obtained using the following transformation.

\[
\begin{bmatrix}
I_{xx} & I_{xy} & I_{xz} \\
I_{xy} & I_{yy} & I_{yz} \\
Sym. & I_{zz}
\end{bmatrix}
= [T]^T
\begin{bmatrix}
\bar{I}_{xx} & \bar{I}_{xy} & \bar{I}_{xz} \\
\bar{I}_{yy} & \bar{I}_{yz} & \bar{I}_{xz} \\
Sym. & \bar{I}_{zz}
\end{bmatrix}
[T]
\]

where \([T]^T\) denotes the transposition of the matrix \([T]\). Once the mass moments and products of inertia at position B are given, the energy restitution coefficient can then be calculated.
5.3.3.2 Description of the experiments

Figures 5.18 and 5.19 show the drop test apparatus and setup. A vacuum pump is used to hold a grain. A high-speed camera (Phantom v4.1) was used to record the motion of the grain immediately before and after impact. This camera system provides a maximum recording speed of 1000 images per second using the sensor's full 512×512 pixel array. By reducing the image size to 32×128 pixel array, it can offer a speed of up to 32000 pps. An image software MA Studio 3.2.1 (Alliance Vision, 2002) was employed to extract data from digitised image sequences captured with the high-speed camera.
Figure 5.18 Drop test apparatus setup

Figure 5.19 Drop test apparatus
5.3.3.3 Test results and discussions

Drop tests were carried out to determine the restitution coefficient for glass beads and Garst corn grains on an acrylic plate. The drop heights for glass beads and Garst corn grains are 290 and 390 mm respectively, thus corresponding to the impact velocities 2.39 and 2.77 m/s. Five samples were tested. Each test was repeated 10 times for glass beads and 15 times for Garst corn grains.

The mean value and variation coefficient of normal restitution coefficient for glass beads are given in Table 5.9. Detailed measurements can be found in Appendix A (Table A.26). Since the glass beads (diameter =10 mm, diameter tolerance = ±0.5 mm) always rebound almost vertically because of sphericity, the normal restitution coefficient approaches the resultant and energy restitution coefficients. It can be seen from Table 5.9 that the coefficient of variation is only 2.2%.

The mean and variation coefficients for normal and resultant restitution coefficients for Garst corn grains are given in Table 5.9. Detailed measurements can be found in Appendix A (Table A.27 and A.28). In the data analysis, only Garst corn grains which rebounded with minimal rotation were selected. It can be seen from Table 5.9 that the variation coefficients for both normal and resultant restitution coefficients are less than 10% and the mean value of the normal restitution coefficient (0.589) is close to the mean value of the resultant restitution coefficient (0.593).

Drop tests were also carried out to determine the restitution coefficient for ellipsoidal medicine tablets on an acrylic plate to illustrate the proposed method. Figure 5.20 shows typical consecutive images (taken from the high-speed camera) of the medicine tablet motion during drop test. Each image has two pictures of the particle, the left being the reflection from the 45° mirror. Images a, b and c show the motion of the medicine tablet before impact, whilst images d, e, f, g, h, i, j, k and l show the rebound motion. The tablet showed only translation (no rotation) before impact, but it spun significantly in addition to some translation immediately after impact due to the tangential contact force induced during the process of collision. The mean and variation coefficients for the normal, resultant and energy restitution coefficients are
given in Table 5.9. Detailed measurements can be found in Appendix A (Table A.29). All three kinds of definition were used and the corresponding results were compared. From Table 5.9, the mean value of the normal and resultant restitution coefficients are 0.265 and 0.272 with the variation coefficients of 97.5% and 93.2%, respectively. However, the variation coefficient for energy restitution coefficient is less than 10% and the mean value is 0.687. These results seemed to be repeatable and indicated that for a fixed drop height (or constant impact velocity), the energy lost may be relatively constant, thus producing repeatable energy restitution coefficients. The rebound energy can be transformed to a combination of translation energy and rotation energy depending on the impact condition and the particle’s inertial properties. This measurement illustrates the need to include particle rotation in the determination of restitution coefficient for non-spherical particles which is not easy to measure and evaluate properly. The method described here allows the restitution coefficient for irregularly shaped particles to be determined accurately.

Table 5.9 Restitution coefficients for different type grains

<table>
<thead>
<tr>
<th>Grain type</th>
<th>Glass bead</th>
<th>Garst corn</th>
<th>Medicine tablet</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normal restitution Coefficient</td>
<td>0.793</td>
<td>0.589</td>
<td>0.265</td>
</tr>
<tr>
<td>CoV (%)</td>
<td>2.2</td>
<td>7.8</td>
<td>97.5</td>
</tr>
<tr>
<td>Resultant restitution Coefficient</td>
<td>0.593</td>
<td></td>
<td>0.272</td>
</tr>
<tr>
<td>CoV (%)</td>
<td>7.5</td>
<td></td>
<td>93.2</td>
</tr>
<tr>
<td>Energy restitution Coefficient</td>
<td></td>
<td></td>
<td>0.687</td>
</tr>
<tr>
<td>CoV (%)</td>
<td></td>
<td></td>
<td>3.4</td>
</tr>
</tbody>
</table>
Figure 5.20 Consecutive images of a drop test for a medicine tablet (Part I). Before impact: a, b and c. After impact: d, e, f, g, h, i, j, k and l
Figure 5.20 Consecutive images of a drop test for a medicine tablet (Part II). Before impact: a, b and c. After impact: d, e, f, g, h, i, j, k and l
5.4 Summary

The methodologies and experimental apparatuses to measure the main particle parameters namely Young's modulus, friction coefficient and restitution coefficient for DEM models have been presented in this chapter. Measurements of the physical and mechanical properties for samples of corn, wheat and glass beads have been reported. The following conclusions can be drawn:

1. A specified number of grains were weighed to determine the mean and variation coefficient of the mass of single grains. The linear dimensions of the grains were first measured directly using digital callipers. More accurate description of the grain shape was obtained from 3D laser scans. The specific weight was calculated according to the mass and volume of grain samples. In addition, the loose and dense bulk densities of grains were also determined.

2. The Young's modulus of individual corn grains was evaluated using two methods. First, the modulus was determined from the single particle indenter compression test according to the ASAE Standard. This method was found to be not suitable for grains that are not sufficiently flat at the region of contact. Second, the modulus was evaluated from a rigid platen compression test together with the radii of curvature measured using a 3D scanner. This proposed method has been shown to be stable during the single particle compression test and can be applied to any irregularly shaped agricultural grains, regardless of size and shape.

3. A sliding test apparatus was devised to measure the static particle-surface friction coefficients. This sliding friction test has been shown to be stable and reproducible.

4. A drop test apparatus has been built to determine the particle-surface restitution coefficient. The various definitions for the restitution coefficient have been outlined and discussed. A new methodology to determine the restitution coefficient for irregularly shaped particles has been presented.
5. The physical and mechanical properties for samples of corn, wheat and glass beads are listed in Tables 5.1-5.10. Detailed measurements can be found in Appendix A. This provides a database of measurements that can be used for simulations of grain dynamics.
Chapter 6

Comparison between DEM simulations and physical experiments

6.1 Introduction

This chapter describes the comparison between DEM simulations and physical experiments. The loading scenarios include silo/cylinder filling, confined compression, rod penetration and silo discharge through an orifice, as shown in Figure 6.1. Both spherical (glass beads) and non-spherical (corn grains) particles were studied. Spherical particles have been very extensively studied with a huge amount of information existing in the literature, so modelling spherical particles serves to link into the existing literature and by comparing with the corn grain simulations, highlight the influence of particle shape on DEM. The mechanical and geometrical properties for the particles were measured as described in Chapter 5 for use in the DEM computations.

This chapter begins the description of the experimental setups. The key features for DEM modelling of these experiments are then presented before comparison is made for each of the loading scenario studied.
6.2 Physical experiments

6.2.1 Silo filling (space filling)

The silo filling test was to investigate the packing density of a granular solid in a cylinder. A fixed mass of the test solid was placed into the cylinder in a distributed manner through a sieve placed at the top of the cylinder. The filling height was measured to give the bulk density which can be compared with DEM results. The test was performed several times to check repeatability.
6.2.2 Confined compression test

The confined compression test (Figure 6.2) was designed to investigate the mechanical response of a granular material under vertical loading and the load transfer to the containing walls. The apparatus was modified from the K₀ tester (Masroor et al., 1987) available in the Particulate Solids Laboratory at the University of Edinburgh. A load was applied to a granular assembly contained in the cylinder through a top platen driven by an INSTRON machine at a constant displacement rate of 1.5 mm/min. The applied load and vertical displacement were measured using the INSTRON machine. The force transmitted to the walls was measured using four strain gauges equally spaced around the cylinder walls in both circumferential and axial directions. The vertical force transmitted to the bottom platen was measured by the bottom load cell. The lateral pressure ratio \( K \) and the bulk wall friction coefficient \( \mu_{\text{bulk}} \) can be determined approximately using Eqs. (6.1-6.2) respectively.

\[
K = \frac{\sigma_H}{\sigma_v} \quad (6.1)
\]

\[
\mu_{\text{bulk}} = \frac{\tau}{\sigma_H} \quad (6.2)
\]

where \( \sigma_v \) is the average vertical stress determined from the average of the top and bottom load cell readings; \( \sigma_H \) is the mean horizontal stress at the strain gauge level, determined from the strain gauge readings; and \( \tau \) is the average shear stress calculated from the difference between the top and bottom load cell readings. These stresses are expressed as

\[
\bar{\sigma}_v = \frac{2(F_T + F_B)}{\pi D^2(1 + \nu_w)} \quad , \quad \sigma_H = \frac{2\mu E_w (\varepsilon_\theta + \nu_w \varepsilon_a)}{D(1 - \nu_w^2)} \quad , \quad \bar{\tau} = \frac{F_T - F_B}{\pi Dh(1 - \varepsilon_v)} \quad (6.3)
\]

In Eq. (6.3): \( D \), \( t \), \( E_w \) and \( \nu_w \) are the diameter, thickness, Young’s modulus and Poisson’s ratio of the cylinder respectively; \( \varepsilon_\theta \), \( \varepsilon_a \) are the average hoop strain and axial strain of the cylinder at the measuring points respectively; \( F_T \), \( F_B \) are the
applied load at the top platen and the measured force at the bottom platen respectively; \( \bar{\varepsilon}_v \) is the mean vertical strain and \( h \) is the height of the granular solid.

The diameter, thickness, and height of the cylinder are 145 mm, 3.33 mm and 380 mm respectively. The average heights of the test specimens for glass beads and corn grains are 185 mm and 141 mm respectively. The strain gauges in the glass bead and corn grain tests were located at 94 mm and 76 mm from the bottom of the bulk solid respectively. This interpretation of the test relies on: (a) the cylinder wall is fairly thin; (b) the strains measured at different points around the circumference are nearly equal. Figure 6.3 shows the hoop strain and axial strain versus time in one of the four confined compression tests (Glass bead Test_4) for glass beads. A corresponding set of strain data (Corn grain Test_1) for corn grains are shown in Figure 6.4.

The strain measurements showed significant variation around the circumference, with the largest variation observed in the axial strain for corn grains. Under small loads, the strain readings for glass beads varied less around the circumference. Further investigation is needed to explore the cause(s) of this non-uniformity which may come from a number of sources. The strain variation around the circumference implies that the membrane theory of shell used to infer the mean horizontal stress in the solid is not totally valid. As a first approximate analysis, only the average of the four strain readings is used in the analysis presented in Section 6.5.
Attached to an INSTRON machine

Top view

Side view

a) Confined compression test setup

b) Confined compression test for glass beads

c) Confined compression test for corn grains

Figure 6.2 Confined compression test
Figure 6.3 Strain gauge readings for glass bead confined compression test
Figure 6.4 Strain gauge readings for corn grain confined compression test
6.2.3 Rod penetration test

The penetration test was designed to evaluate the resistance of granular bulk to penetration of a moving object and the dynamic force transmission to a contact surface. The experimental design is depicted in Figure 6.5. The force and displacement of a rod were monitored using an INSTRON machine as the rod was pushed into a granular bulk at a constant displacement rate of 50 mm/min.

6.2.4 Silo discharge test

The silo discharge experiment is illustrated in Figure 6.6. This experiment was conducted by releasing grains through a circular orifice of a flat-bottomed silo onto a flat surface. The angle of repose of the heap was measured.

Table 6.1 presents a summary of the physical experiments, indicating the test methods and test observations.

<table>
<thead>
<tr>
<th>Physical experiments</th>
<th>Method</th>
<th>Measured data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Silo/cylinder filling</td>
<td>Filling a cylindrical container with a specified mass of grains.</td>
<td>Filling height.</td>
</tr>
<tr>
<td>Confined compression test</td>
<td>Compressing a grain bulk confined in a thin-walled cylinder by a top platen using an INSTRON machine. The vertical transmitted force to the bottom platen was measured using another load cell. The radial force was measured using strain gauges fixed to the cylinder walls.</td>
<td>Force-displacement response, force applied to the bottom load cell, axial and hoop strains on the cylinder wall at the measuring point.</td>
</tr>
<tr>
<td>Rod penetration test</td>
<td>Pushing a cylindrical rod with a spherical cap into a grain bulk at a constant displacement rate 50mm/min.</td>
<td>Dynamic force transmission to a rod, force-displacement response.</td>
</tr>
<tr>
<td>Silo discharge test</td>
<td>Emptying grains from a flat-bottomed silo onto a flat receiving pan.</td>
<td>Angle of repose.</td>
</tr>
</tbody>
</table>
IF

Force acting on the rod

Container

Grain bulk

Cylindrical rod: diameter = 25 mm length = 232.5 mm

Spherical cap

a) Rod penetration: test setup and rod dimensions

b) Rod penetration test for glass beads
c) Rod penetration test for corn grains

Figure 6.5 Rod penetration test
a) Silo discharge test setup

b) Silo discharge test for glass beads
c) Silo discharge test for corn grains

Figure 6.6 Silo discharge test
6.3 Discrete element modelling of physical experiments

For all DEM simulations, Hertz-Mindlin no-slip (Tsuji et al., 1992) contact model with damping and a frictional slider in the tangential direction was used, as shown schematically in Figure 3.1. A multiplier of 0.20 (20%) was applied to the computed critical time step for all DEM simulations. This value was chosen to achieve numerical stability without increasing computational cost (O'Sullivan and Bray, 2004c). The numerical samples were prepared by filling a cylindrical container (diameter = 145 mm, length = 300 mm) with 3591 glass beads and 4672 corn grains in each set of computations. Particle size variation was not considered in these numerical calculations. The corn particle was represented using overlapping spheres (Favier et al., 1999; ITASCA, 2003) to match the measured average major, intermediate and minor dimensions. A 4-sphere representation (Figure 6.7) was chosen initially to manage the computational effort required for the large number of simulations planned. Subsequently, the 4-sphere representation was adhered to because it appeared to be sufficient to give satisfactory predictions.

It is generally known that the bulk behaviour of a particulate assembly can be sensitive to its packing structure. Care should therefore be taken in the initial particle generation to simulate as closely as possible the packing structure that would prevail in the real situation. Whilst the DEM software has the capability to simulate the filling procedure used in this study, i.e. raining through a sieve, the computational effort would be huge and impractical to conduct. There is also the issue of whether
this level of modelling is necessary to achieve a satisfactory prediction. In this study, all particles were generated in a regular grid and “switched on” from the start. The effect of this approximation is further explored using different initial particle positions and will be discussed in Section 7.2.

The particles are positioned in layers starting from the base, at 1.50\(d\) centre to centre for glass beads and 1.01\(d\) centre to centre for corn grains as shown in Figure 6.8 (\(d\) = major diameter of the particle). They were all assigned an initial velocity of 2.56 m/s which corresponds to the drop height used in the experiments where the particles were placed in a sieve at a height of 335 mm and allowed to “rain” through the sieve into the cylinder. They were then allowed to fall under gravity to achieve the initial filled state. The particles were deemed to have settled down when the kinetic energy of the system approached zero (<10\(^{-8}\) J) and the mean unbalanced force approached zero (<10\(^{-6}\) N), compared to a single glass bead weight of 1.3\(\times10^{-2}\) N and a single corn grain weight of 4.2\(\times10^{-3}\) N.

After achieving the filled state, the confined compression was simulated by adding a top platen with a displacement rate of 50 mm/min. The rod penetration was simulated by adding a steel rod with a displacement rate of 50 mm/min. The silo discharge was simulated by removing some triangular elements to create an orifice on the bottom platen. Discharging from three orifice sizes was simulated to investigate granular flow. Orifice sizes are 0.2D, 0.4D and 0.6D (D = 145 mm, diameter of the cylinder) respectively and the distance between the outlet and receiving pan is 150 mm. Input parameters for the glass beads and corn grains are listed in Tables 6.2 and 6.3 respectively. Sigmund Lindner stated in their literature that the glass beads they provided have a Poisson’s ratio of 0.22 but did not indicate how it was determined. The range of the Poisson’s ratio for glass beads given by Gere and Timoshenko (1991) is 0.20–0.27. The value of 0.22 from the manufacturer was adopted in this study. The value of the Poisson’s ratio for corn grains was assumed to be 0.4 in the ASAE standard which is adopted in this study. Individual particle-particle friction and restitution coefficient measurement has rarely been attempted before in irregularly shaped agricultural grains. The values for the inter-
particle friction and restitution coefficients were first assumed to be the same as those for the particle-surface friction and restitution coefficients. The sensitivity of the assumed values for the inter-particle friction and particle-rod friction was explored, which will be discussed in Section 7.4 and 7.5, respectively. The typical input files for both EDEM and PFC3D codes can be found in Appendix D.

Table 6.2 Input parameters for glass beads

<table>
<thead>
<tr>
<th>Properties</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter</td>
<td>10</td>
<td>mm</td>
</tr>
<tr>
<td>Density</td>
<td>2530</td>
<td>kg/m$^3$</td>
</tr>
<tr>
<td>Young's modulus</td>
<td>41</td>
<td>GPa</td>
</tr>
<tr>
<td>Poisson's ratio (from Sigmund Lindner)</td>
<td>0.22</td>
<td></td>
</tr>
<tr>
<td>Static friction coefficient (glass bead-acrylic)</td>
<td>0.24</td>
<td></td>
</tr>
<tr>
<td>Static friction coefficient (glass bead-glass bead)</td>
<td>0.24</td>
<td></td>
</tr>
<tr>
<td>Restitution Coefficient (glass bead-acrylic)</td>
<td>0.79</td>
<td></td>
</tr>
<tr>
<td>Restitution Coefficient (glass bead-glass bead)</td>
<td>0.79</td>
<td></td>
</tr>
<tr>
<td>Number of glass beads</td>
<td>3591</td>
<td></td>
</tr>
</tbody>
</table>

Table 6.3 Input parameters for corn grains

<table>
<thead>
<tr>
<th>Properties</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Major dimension</td>
<td>10.11</td>
<td>mm</td>
</tr>
<tr>
<td>Intermediate dimension</td>
<td>9.11</td>
<td>mm</td>
</tr>
<tr>
<td>Minor dimension</td>
<td>6.69</td>
<td>mm</td>
</tr>
<tr>
<td>Density</td>
<td>1280</td>
<td>kg/m$^3$</td>
</tr>
<tr>
<td>Young's modulus</td>
<td>1660</td>
<td>MPa</td>
</tr>
<tr>
<td>Poisson's ratio (ASAE)</td>
<td>0.4</td>
<td></td>
</tr>
<tr>
<td>Static friction coefficient (corn grain-acrylic)</td>
<td>0.34</td>
<td></td>
</tr>
<tr>
<td>Static friction coefficient (corn grain-corn grain)</td>
<td>0.34</td>
<td></td>
</tr>
<tr>
<td>Restitution Coefficient (corn grain-acrylic)</td>
<td>0.59</td>
<td></td>
</tr>
<tr>
<td>Restitution Coefficient (corn grain-corn grain)</td>
<td>0.59</td>
<td></td>
</tr>
<tr>
<td>Number of corn grains</td>
<td>4672</td>
<td></td>
</tr>
</tbody>
</table>

6.4 Comparison for silo filling

Figure 6.8 illustrates example snapshots of particle filling for glass beads and corn grains respectively. Tables 6.4 and 6.5 compare filling densities between DEM and experiments. The filling densities from DEM simulations are calculated based on applied vertical stress of 1.3 and 5.0 kPa. It can be seen that DEM predicted lower bulk densities than experiments (~8% lower for glass beads and ~17% lower for corn grains). The possible sources of the discrepancy are listed as follows:

1. The particles are mono-sized in the DEM model and particles of different sizes pack differently. The diameter of glass beads has a mean of 10.0 mm with a tolerance of ±0.5 mm. The linear dimensions for corn grains have mean values of 10.1, 9.1 and 6.7 mm with CoVs of 8%, 5% and 17% in length, width and height respectively. The natural size variation should allow
the granular bulk to pack more densely, hence producing a higher filling density.

2. The assumed inter-particle friction may not be representative of the actual value. A lower inter-particle friction will lead to denser packing.

3. The inter-particle stiffness has been related to the curvature of the idealised particle instead of the small bumps (asperities) through which particles probably often contact each other.

4. The Hertz-Mindlin elastic frictional based spring-dashpot contact model is not be particularly suited to soft agricultural grains where plastic deformation at contact points is expected to occur under loading.

5. In the case of corn, the rather crude 4-sphere approximation was used to represent the particle shape of smooth corn grains.

There may be other reasons, but lack of time prevented any further exploration.

![Figure 6.8 Example snapshots of silo filling](image)

**Figure 6.8** Example snapshots of silo filling

**Table 6.4** Comparison of filling densities between simulation and experiment for glass beads

<table>
<thead>
<tr>
<th>Glass beads</th>
<th>DEM</th>
<th>Test average</th>
<th>Test CoV (%)</th>
<th>Difference (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bulk density (kg/m³) (applied vertical stress = 1.3 kPa)</td>
<td>1442</td>
<td>1560</td>
<td>0.3</td>
<td>8</td>
</tr>
<tr>
<td>Bulk density (kg/m³) (applied vertical stress = 5.0 kPa)</td>
<td>1445</td>
<td>1560</td>
<td>0.3</td>
<td>7</td>
</tr>
</tbody>
</table>

**Table 6.5** Comparison of filling densities between simulation and experiment for corn grains

<table>
<thead>
<tr>
<th>Corn grains</th>
<th>DEM</th>
<th>Test average</th>
<th>Test CoV (%)</th>
<th>Difference (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bulk density (kg/m³) (applied vertical stress = 1.3 kPa)</td>
<td>713</td>
<td>859</td>
<td>0.2</td>
<td>17</td>
</tr>
<tr>
<td>Bulk density (kg/m³) (applied vertical stress = 5.0 kPa)</td>
<td>717</td>
<td>859</td>
<td>0.2</td>
<td>17</td>
</tr>
</tbody>
</table>
The following procedure was used to calculate the normal wall pressure distribution. Firstly, the height of the cylindrical wall was divided into a certain number of segments. For silo filling and confined compression of glass beads in Chapter 6, a total of 8 ring segments were used, as shown in Figure 6.9 (a). For all other simulations that were performed in Chapter 6, Chapter 7 and Chapter 8, a total of 15 ring segments were used to increase the resolution of the pressure calculation, as shown in Figure 6.9 (b). In the former case, the height for each segment is 37.5 mm (3.75 times of the diameter of glass beads), whilst the height for each segment in the later cases is 20 mm (approximately twice the major diameter of the particles).

In EDEM, the particle-wall contact output consists of the resultant force and moment at the centroid of each triangular wall element. The normal force and vertical shear force applied on each wall element were calculated by using coordinate transformation. The total normal force and total vertical shear force for each segment were then determined from the summation of individual normal force and vertical shear force for each wall element within the segment. The normal pressure for a segment is then obtained by dividing the total normal force by the surface area of the segment. In PFC, the particle-wall contact output directly provides the normal force and vertical shear force. The total normal force and total vertical shear force for each segment were determined from the summation of individual normal force and vertical shear force for each particle-wall contact within the segment. Similarly, the normal pressure for a segment is then obtained by dividing the total normal force by the surface area of the segment. A similar procedure was used to compute the vertical wall traction from the total contact vertical shear force in each segment.

This first level calculation computes the axisymmetric component of the wall pressure. It has been noted that the local variations in the pressure distribution is rather dependent on the size of ring segment used to compute the average pressures, so that as the number of segments increases, a greater degree of local variations can be expected (Holst et al, 1999). The influence of segment size will be explored in more details in the post-thesis research in preparation for journal publications. Further more detailed calculation can also be performed to look at how the pressure
might vary around the circumference by dividing the circumference into further sub-segments.

Figure 6.10 shows the normal wall pressure distribution acting on the cylindrical wall at the end of filling. The pressures acting on the container can be evaluated from the DEM boundary contact forces. This pressure distribution may be compared with the one-dimensional theory of Janssen for silo wall pressure (Janssen, 1895; Ooi and Rotter, 1990; Rotter, 2001):

\[ P_z = \frac{Dy}{4\mu} (1 - e^{-z/z_0}) + K q_r e^{-z/z_0} \]  

(6.4)

\[ z_0 = \frac{D}{4\mu K} \quad q_r = \frac{F_r}{\pi D^2} \]  

(6.5)

where \( K \) is the lateral pressure ratio, \( \mu \) is the wall friction coefficient, \( \gamma \) is the bulk density, \( z_0 \) is the Janssen reference depth and \( q_r \) is the mean vertical pressure that may be applied at the top boundary (\( z=0 \)). The predicted \( K \) and \( \mu_{bulk} \) can be estimated from the boundary forces in the DEM results. The Janssen best fit curves for both glass beads and corn grains indicate that wall friction is effectively zero in the DEM calculations. The pressure distributions for both solids were predicted to increase almost linearly with depth, suggesting that very little bulk wall friction is generated during filling in this small cylinder. Given that the cylinder diameter is 145 mm and the filling heights were 185 mm and 141 mm respectively for the glass beads and corn grains, the filling aspect ratios resemble one of a squat silo where the pressure distribution can be quite linear. Even so, the total lack of wall friction in these DEM calculations needs further investigation especially on the question of whether DEM can predict the silo arching phenomenon. In the confined compression simulation following on from the filling simulation, wall friction was increasingly generated under additional vertical loading, with the corn grain simulation approaching the limiting particle-wall friction coefficient used in the simulation.
a) A total of 8 ring segments were used for glass bead silo filling and confined compression simulation

b) A total of 15 ring segments were used for all other simulations

**Figure 6.9** The ring segments for computing the normal wall pressure and vertical wall traction
Figure 6.10 Normal wall pressure distribution at the end of filling

a) Glass beads

b) Corn grains
6.5 Comparison for confined compression

In earlier trials of the experiment, it was found that several particles protruded significantly from the overall surface after filling and this occurrence significantly affected the stability of the vertical compression, especially for the stiff glass beads. Thus for the final experiments reported in this thesis, several significantly protruding particles on the top surface were carefully picked and rearranged to make the top surface flatter, before the top platen was gently put on the bulk solid. In the DEM calculations, the top platen was directly applied on the bulk solid after the particles were deemed to have settled down (as described in Section 6.3). The lid was made of Delrin to minimise friction and backed by a stiffening aluminium plate so that the lid can be deemed to be rigid. In the DEM simulation, the measured friction coefficient for particle-acrylic plate was adopted.

Figure 6.11 illustrates example snapshots of confined compression for glass beads and corn grains respectively. Figures 6.12 (a) and (b) compare the load-displacement responses between DEM computation and four confined compression tests for glass beads and corn grains respectively. The overall trend of increasing stiffness as vertical load increases is as expected. Studying the simulation images showed that at the initial stage of the DEM simulations, particles rearrangement occurred primarily near the top surface in response to the loading platen coming down. Several sudden falls in force occurred later in the loading in both experiments and simulations for the glass beads (Figure 6.12a). For the corn grains, no sudden drop occurred in the experiments but one small drop was observed in the DEM simulation (Figure 6.12b). This may be due to collapse of some local network of forces (i.e. some local reorganisation of force chains) which leads to a sudden drop in vertical movement and hence the sudden drop in the vertical force. A careful study of microstructure of the particle assembly from the DEM output including force chain, coordination number etc will shed light on the cause(s). This work is mentioned in the Conclusion Chapter as an area worthy of further research.
The slope of the lines in four tests and DEM result were calculated for both materials by using linear regression and considering the data after 200 N vertical forces, as shown in Figure 6.12. The slope in tests has mean values of 1641 and 627 N/mm with CoVs of 8.2% and 3.0% for glass beads and corn grains respectively, whilst the slope in DEM has mean values of 4987 and 1348 N/mm for glass beads and corn grains respectively. Although each physical test followed the same filling procedure, the results show that at the initial stage when the forces are small, the loading response can vary significantly from test to test. This suggests that the natural variation in initial packing in each experiment can give significantly different loading responses at low stresses. After this initial confinement (say after 200 N vertical force), the loading responses were largely parallel to each other, indicating that each test assembly converged to a repeatable loading response at higher confining pressures. The DEM predicted response appears to be stiffer than the experimental observations, which is not surprising for the following reasons:

1. The DEM model does not take into account the flexibility of the cylindrical walls (which was necessary to achieve a measurable strain to determine the wall loading), thus producing stiffer loading response.
Figure 6.12 Load-displacement responses during confined compression
2. The particle contact stiffness is sensitive to radii of curvatures at the point of contact (see Eq. 5.19). Representing a corn grain using overlapping spheres means that the radii of curvature in the model can be quite different from the actual radii of curvature in contacts on a real corn grain. This significant influence on the contact stiffness needs more careful thinking and consideration.

3. The Hertz-Mindlin elastic frictional contact model (with an additional damper) was used for all DEM simulations. However, soft corn grains can be expected to have a much more complex contact interaction with non-linear elasto-visco-plastic response under loading, which can be expected to produce a softer response under increasing load. Developing a more appropriate contact model for soft grains may help to improve the predict the bulk stiffness.

4. Uniform spheres can sometimes get into a crystalline formation which does not normally happen in a real system. Additional simulations in Chapter 7 to explore particle packing by setting up rhombic and face-centred-cubic (FCC) packing of spheres show how uniform spheres can get into packing structure that gives a significantly different bulk response. DEM simulations of perfect and uniform spheres often show large particle rotations, which again would be much reduced in the real glass beads due to the natural size variation and surface unevenness. These all points to a greater discrepancy between DEM simulation of perfectly uniform spheres and the experiments on not-so-perfect glass spheres.

Figure 6.13 shows the force transmission onto the bottom platen during compression. Both the experimental and numerical results show the force acting on the bottom platen increases linearly with the applied vertical force. The physical tests show that only 50% of the applied load reached the bottom platen for the glass beads compared with 65% for the corn grains. The DEM produced excellent predictions of the force transfer to the bottom platen during compression for both glass beads and corn grains.

Figure 6.14 shows the development of the normal wall pressures during vertical compression for both materials. The effect of vertical compression can be evaluated from the extended Janssen equation with the inclusion of an applied vertical stress at
z=0 (Eq. 6.4). These are also plotted in Figure 6.14 for comparison, using $K$ and $\mu_{\text{bulk}}$ derived from the DEM results. The increase of normal wall pressures during vertical compression matches the Janssen equation reasonably well away from boundaries. Since Janssen is a one-dimensional theory that does not take into account the top and bottom boundary conditions, there is significant mismatch with the simple Janssen equation especially towards the boundaries. Friction is generated between the platens (top and bottom) and the particles during vertical loading in the experiments and DEM simulations, thus affecting the wall pressure near the boundaries.
Figure 6.13 Force transmission onto the bottom platen during confined compression
Figure 6.14 Normal wall pressure during confined compression
The ratio of vertical traction to normal pressure at any point on the wall gives an indication of the "coefficient of mobilised bulk wall friction" at that point. Figure 6.15 shows the mobilised bulk wall friction against the height above the base for both materials. It can be seen that as vertical load increases, the bulk wall friction is increasingly being mobilised. In Figure 6.15 (a), the mobilised wall friction at the four instants calculated are within the range of 0.07~0.17 for the glass beads, significantly smaller than the input particle-wall friction coefficient of 0.24. This is in agreement with previous studies (Rotter et al., 1998) showing significantly smaller macroscopic friction than the inter-particle microscopic friction for a spherical assembly. For the corn grains, a higher mobilized bulk wall friction is achieved with values of 0.21~0.31 when the vertical force is close to 1000 N (this compares with input friction coefficient of 0.34). The main reason may be that since glass beads are much stiffer than corn grains, they do not generate sufficient slip displacement against the wall, resulting in much smaller bulk wall friction mobilisation (the influence of particle stiffness on the bulk behaviour was explored by reducing the assumed value of shear modulus G from the measured value G₀ to 0.01G₀ and 0.0001G₀ for both materials and will be presented in Section 7.3). The tendency for perfect spheres to rotate more as compared to non-spherical particles may also contribute to the smaller macroscopic friction.
Figure 6.15 Mobilized bulk wall friction coefficient during confined compression
The lateral pressure ratio $K$ was evaluated from the experimental data using Eq. (6.1) and plotted against the DEM prediction in Figure 6.16. The experimental results are reasonably repeatable for each material, showing a trend of the $K$ value increasing and reaching a stable value of $\sim0.4$ for glass beads and $\sim0.35$ for corn grains, with a larger scatter for the glass beads. It should be noted that the evaluation of lateral pressure ratio $K$ is only approximate here since the mean vertical stress was calculated from the average of top and bottom platen forces (Eq. 6.3) for both the DEM simulations and experiments and the normal pressure came from measurement at the strain gauge level in the experiment and from boundary forces in the DEM simulations. The DEM prediction for the corn computation is in excellent agreement but for the sphere assembly, DEM predicts a much larger $K$ value of $\sim0.72$. The over-prediction of $K$ value matches the finding from previous studies for 2D circular disks (e.g. Rotter et al., 1998; Holst et al., 1999).

Figure 6.17 shows the mobilized bulk wall friction coefficient $\mu_{\text{bulk}}$ against the applied load and compares the DEM prediction with the experiments. Following the same reasoning for the lateral pressure ratio $K$, the comparison between DEM simulation and experiments is only approximate. It can be seen that there is a reasonable match for the corn grains, but DEM predicts a much smaller $\mu_{\text{bulk}}$ value of $\sim0.15$ for the sphere assembly.
Figure 6.16 Lateral pressure ratio versus top applied load

(a) Glass beads

(b) Corn grains
Figure 6.17 Mobilized bulk wall friction coefficient versus top applied load
6.6 Comparison for rod penetration

Figure 6.18 illustrates example snapshots (global view and diametral view) of rod penetration for glass beads. The experimental load-displacement responses for the rod penetration into glass beads and corn grains are shown in Figure 6.19. These are compared with DEM computations that were performed with particle shear modulus $G_0$ decreased to $0.01G_0$ to reduce computational effort. The measured force fluctuated significantly during penetration into each material, but the average trend is repeatable with the corn grains giving a larger resistance to penetration than the glass beads. The DEM results also fluctuated in a similar fashion and showed a good quantitative match with the experiments. Reducing particle stiffness did not show any significant effect on the simulation outcomes, but provided considerable speed-up. The effect of particle stiffness on the load-displacement response during rod penetration was explored and will be presented in Section 7.3.

Figure 6.18 Example snapshots of rod penetration
Figure 6.19 Comparison of load-displacement response during rod penetration between experiment and simulation

a) Glass beads

b) Corn grains
6.7 Comparison for silo discharge

Figures 6.20 and 6.21 depict consecutive snapshots of glass bead discharge for orifice size of 0.6D and 0.4D respectively (D is the diameter of the cylinder at 145 mm). The two orifices are 8.7 and 5.8 times the particle size. Colour in the figures is coded for particle velocity: blue=0.00 m/s to green=0.05 m/s to red=0.10 m/s. A study of the velocity field indicates that in the 0.6D case, the flow pattern is mass flow for a major part of the solid during discharge, whilst in the 0.4D case, the flow pattern is also mass flow but at a lower discharge velocity, and it becomes internal funnel flow at some stage during the discharge because of the smaller orifice. In contrast, the 0.2D orifice leads to mechanical arching over the orifice, resulting in no flow. Figure 6.22 shows the mass flow rates versus time for 0.4D and 0.6D orifices with glass beads and corn grains respectively. Away from initial and final stages of discharge, flow rate is independent of the height of solid in the cylinder. Ignoring the trends near the start and the end of each curve, only the relative stable middle region was used to calculate the average flow rate (Figure 6.22). The ranges chosen for calculating the mass flow rates are marked in Figure 6.22, i.e. from point 1 to point 2 for 0.4D case and from point 3 to point 4 for 0.6D case. The mean value and CoV for each mass flow rate calculation are also indicated in the figure. Tables 6.6 and 6.7 show the predicted mass flow rates for different orifices involving glass beads and corn grains. These mass flow rates may be compared with Beverloo formula (Beverloo et al., 1961).

$$W = C \rho_b \sqrt{g(D_o - kd)^{2.5}}$$  \hspace{1cm} (6.6)

where $\rho_b$ is the bulk density of the solid, $g$ the gravity, $D_o$ the diameter of the orifice, and $d$ the diameter of particles. According to Nedderman (1992), the Beverloo constant $C$ may be in the range from 0.58 to 0.64 and the adjustment $k$ should be around 1.5 for spherical particles. It can be seen that predicted mass flow rates compare well with Beverloo formula, with the constant $C$ being closer to 0.64 for glass beads and closer to 0.58 for corn grains, as expected.
Table 6.6 Comparison of mass flow rates between simulation and Beverloo formula for glass beads

<table>
<thead>
<tr>
<th>Outlet diameter</th>
<th>Mass flow rate (kg/sec) (DEM)</th>
<th>Mass flow rate (kg/sec) (Beverloo formula)</th>
<th>Difference (%) C=0.58</th>
<th>Difference (%) C=0.64</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2D</td>
<td>1.047</td>
<td>1.003-1.107</td>
<td>-4.3</td>
<td>5.5</td>
</tr>
<tr>
<td>0.6D</td>
<td>4.002</td>
<td>3.640-4.016</td>
<td>-10.0</td>
<td>0.3</td>
</tr>
</tbody>
</table>

Table 6.7 Comparison of mass flow rates between simulation and Beverloo formula for corn grains

<table>
<thead>
<tr>
<th>Outlet diameter</th>
<th>Mass flow rate (kg/sec) (DEM)</th>
<th>Mass flow rate (kg/sec) (Beverloo formula)</th>
<th>Difference (%) C=0.58</th>
<th>Difference (%) C=0.64</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2D</td>
<td>0.830</td>
<td>0.911-1.005</td>
<td>8.9</td>
<td>17.4</td>
</tr>
<tr>
<td>0.6D</td>
<td>3.185</td>
<td>3.132-3.456</td>
<td>-1.7</td>
<td>7.8</td>
</tr>
</tbody>
</table>

By using the DEM mass flow rates on two outlet diameters, the best fit values of C and k for these runs can be determined from Eq. 6.6. The best fit values of C and k for glass beads are 0.69 and 1.72 respectively, whilst the best fit values of C and k for corn grains are 0.68 and 2.00 respectively. It appears that DEM tends to predict higher values of C and k than the range reported by Nedderman from experimental observations (1992).

Figure 6.23 shows the repose state of glass beads and corn grains at the end of silo discharge tests (0.6D case). The glass beads spread out and did not form any significant pile, whilst the corn grains produced a significant conical pile. The angle of repose was measured on XZ and YZ orthogonal planes using image processing technique applied both to the experiments and to the snapshots from DEM simulations. Table 6.8 shows the measurements from experiment, which gives an average angle of repose of 25.2° (CoV=6%). The DEM simulation for glass beads predicted the same situation as the experiment and did not lead to any conical pile. Corn grain simulation produced a significant conical pile and the angle of repose was calculated at the end of each DEM calculation using imaging process software MA Studio 3.2.1 (Alliance Vision, 2002). The measurements are shown in Table 6.9 and give an average angle of repose of 27.7° (CoV=13%). There is a reasonable agreement between DEM simulations and experiments. The slightly larger angle from DEM calculations should be further investigated.
Table 6.8 Measurement of repose angles from corn discharge test

<table>
<thead>
<tr>
<th>Test</th>
<th>XZ-plane</th>
<th>YZ-plane</th>
</tr>
</thead>
<tbody>
<tr>
<td>No.</td>
<td>Angle_Left</td>
<td>Angle_Right</td>
</tr>
<tr>
<td>1</td>
<td>25.2</td>
<td>26.3</td>
</tr>
<tr>
<td>2</td>
<td>26.8</td>
<td>24.5</td>
</tr>
<tr>
<td>3</td>
<td>25.5</td>
<td>23.8</td>
</tr>
<tr>
<td>Mean (each side)</td>
<td>25.8</td>
<td>24.9</td>
</tr>
<tr>
<td>Standard deviation</td>
<td>0.9</td>
<td>1.3</td>
</tr>
<tr>
<td>CoV (%)</td>
<td>3.4</td>
<td>5.2</td>
</tr>
</tbody>
</table>

Table 6.9 Measurement of repose angles from corn discharge simulation

<table>
<thead>
<tr>
<th>Measurement</th>
<th>XZ-plane</th>
<th>YZ-plane</th>
</tr>
</thead>
<tbody>
<tr>
<td>No.</td>
<td>Angle_Left</td>
<td>Angle_Right</td>
</tr>
<tr>
<td>1</td>
<td>21.9</td>
<td>30.3</td>
</tr>
<tr>
<td>2</td>
<td>26.8</td>
<td>30.9</td>
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<tr>
<td>3</td>
<td>21.0</td>
<td>30.0</td>
</tr>
<tr>
<td>4</td>
<td>21.7</td>
<td>30.4</td>
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<td>5</td>
<td>22.1</td>
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<td>6</td>
<td>23.8</td>
<td>29.4</td>
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<tr>
<td>7</td>
<td>27.2</td>
<td>30.0</td>
</tr>
<tr>
<td>8</td>
<td>22.2</td>
<td>29.6</td>
</tr>
<tr>
<td>9</td>
<td>21.3</td>
<td>30.0</td>
</tr>
<tr>
<td>10</td>
<td>20.5</td>
<td>29.6</td>
</tr>
<tr>
<td>Mean (each side)</td>
<td>22.8</td>
<td>29.9</td>
</tr>
<tr>
<td>Standard deviation</td>
<td>2.4</td>
<td>0.5</td>
</tr>
<tr>
<td>CoV (%)</td>
<td>10.3</td>
<td>1.6</td>
</tr>
</tbody>
</table>

Mean
Standard deviation
CoV (%)
Figure 6.20 Consecutive snapshots during discharging in the case 0.6D (Part I) Colour coded for particle velocity: blue (0.0 m/s), green (0.05 m/s) and red (0.1 m/s)
Figure 6.20 Consecutive snapshots during discharging in the case 0.6D (Part II)
Colour coded for particle velocity: blue (0.0 m/s), green (0.05 m/s) and red (0.1 m/s)
Figure 6.21 Consecutive snapshots during discharging in the case 0.4D (Part I)
Colour coded for particle velocity: blue (0.0 m/s), green (0.05 m/s) and red (0.1 m/s)
Figure 6.21 Consecutive snapshots during discharging in the case 0.4D (Part II) Colour coded for particle velocity: blue (0.0 m/s), green (0.05 m/s) and red (0.1 m/s)
Figure 6.22 Mass flow rate for different outlets during discharging
Figure 6.23 Repose state at the end of discharge test
6.8 Summary

Physical calibration experiments of silo filling, confined compression, rod penetration and silo discharge have been developed and conducted, as presented in this chapter. The corresponding DEM simulations have been conducted and comparison between numerical results and experimental results has been made. The majority showed good to excellent match, providing a quantitative validation for the DEM simulations of the problems studied. Plausible explanations are provided where the match is not as good. More specifically, the following conclusions can be drawn.

1. For glass beads: DEM gave good agreement with experiments for silo filling (normal wall pressure distribution), confined compression (normal wall pressure distribution, load transfer to boundary surfaces), rod penetration (force-displacement response), and silo discharge (mass flow rate), but under-predicted bulk wall friction $\mu_{\text{bulk}}$ and over-predicted lateral pressure ratio $K$. The use of perfect spheres to represent not perfectly spherical glass beads as the probable cause should be explored further.

2. For corn grains: the study shows that 4-sphere representation together with the measured corn properties produced good to excellent match with experiments for silo filling (normal wall pressure distribution), confined compression (normal wall pressure distribution, load transfer to boundary surfaces, and bulk design parameters $K$ and $\mu_{\text{bulk}}$), rod penetration (force-displacement response), and silo discharge (mass flow rate and angle of repose). This provides solid verification that DEM is capable of producing quantitative predictions. The findings suggest that very accurate representation of the non-spherical particle shape may not be necessary to produce satisfactory predictions and capturing the key linear dimensions of a particle may be adequate.

3. The two main DEM simulations that produced larger discrepancies with experiments are filling density (~8% lower for glass beads and ~17% lower for
corn grains) and loading stiffness (stiffer response). Plausible explanations for these have been given in Sections 6.4 and 6.5, respectively.

Further to the above conclusions, it should be noted that there are still many useful results that can be derived from further analyses of this large set of DEM and experimental data. Some further analysis has already begun and will be presented elsewhere at a later stage.
Chapter 7

A study of the influence of DEM input parameters

7.1 Introduction

This chapter describes the investigation of the relative importance of DEM input parameters for producing satisfactory predictions. The investigation explores the influence of particle generation scheme (initial packing structure), particle elastic stiffness, inter-particle friction and particle-boundary friction. The findings from these sensitive analyses give a sound indication on when it might be important to determine a certain property more accurately and when it might not be so important because it does not affect the engineering outcomes. It will provide valuable insight into how particle scale (microscopic) parameters affect the bulk scale (macroscopic) behaviour of a granular solid.

7.2 Particle generation scheme: initial packing structure

The initial state of a particulate system needs to be established for a DEM simulation. Rapid particle generation schemes are often used so as to reduce considerably the computational effort required and these are sometimes not even reported. Since packing structure has a significant influence on the bulk behaviour, it is important to explore how a particle generation scheme adopted might influence the numerical
outcomes. In this study, all particles were generated in a grid pattern and allowed to fall into the cylinder (Figure 6.6). Centre-to-centre spacing between the particles was explored with $1.01d$, $1.50d$ and $2.00d$ ($d =$ major diameter of the particle). For the glass beads, in addition to the particle spacing, special packing arrangements (i.e. face-centered-cubic (FCC), rhombic and random) were also investigated. Figure 7.1 shows two orthogonal views of uniform spheres with FCC and rhombic packings.

**Figure 7.1** Orthogonal views of uniform spheres with FCC and rhombic packings (a, b, d and e are cited from O'Sullivan and Bray, 2004c)
Tables 7.1 and 7.2 show the predicted bulk densities for the different particle generation schemes for glass beads and corn grains respectively. For corn grains, three different particle spacings only resulted in DEM bulk density variation of ±2% with a mean of 730 kg/m³, indicating that non-spherical particles may be less sensitive to how the particles are generated as long as some freedom of settling down is permitted. For glass beads, particle spacing of 1.01d, 1.50d and 2.00d resulted in DEM bulk density variation of ±4% with a mean of 1490 kg/m³. FCC/Rhombic/random packing resulted in DEM bulk density variation of ±7% with a mean of 1535 kg/m³. There is thus a larger density variation for glass beads, probably because uniform spheres can get into specific packing structures, giving a larger variation in filling density.

Table 7.1 Filling densities for different particle generations of glass beads

<table>
<thead>
<tr>
<th>DEM and test results</th>
<th>Bulk density (kg/m³)</th>
<th>Vertical stress = 1.33 kPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.01d separation</td>
<td>1549</td>
<td></td>
</tr>
<tr>
<td>1.50d separation</td>
<td>1442</td>
<td></td>
</tr>
<tr>
<td>2.00d separation</td>
<td>1466</td>
<td></td>
</tr>
<tr>
<td>Random generation</td>
<td>1419</td>
<td></td>
</tr>
<tr>
<td>FCC packing</td>
<td>1583</td>
<td></td>
</tr>
<tr>
<td>Rhombic packing</td>
<td>1603</td>
<td></td>
</tr>
<tr>
<td>Test results</td>
<td>1560</td>
<td></td>
</tr>
</tbody>
</table>

Table 7.2 Filling densities for different particle generations of corn grains

<table>
<thead>
<tr>
<th>DEM and test results</th>
<th>Bulk density (kg/m³)</th>
<th>Vertical stress = 1.33 kPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.01d separation</td>
<td>713</td>
<td></td>
</tr>
<tr>
<td>1.50d separation</td>
<td>730</td>
<td></td>
</tr>
<tr>
<td>2.00d separation</td>
<td>747</td>
<td></td>
</tr>
<tr>
<td>Test results</td>
<td>859</td>
<td></td>
</tr>
</tbody>
</table>

Figure 7.2 shows the force on the bottom platen during confined compression of glass beads for the different particle generation schemes. Spacings of 1.50d and 2.00d both matched the experimental results, but the spacing of 1.01d where particles were generated almost touching one another produced a larger force on the bottom platen. It appears that as long as there is sufficient separation between particles to allow the packing structure to form, this method of switching on all particles can work well.
Figure 7.3 shows the force on the bottom platen during confined compression of glass beads for three specially generated packing structures i.e. FCC (cubic close), rhombic (hexagonal close) and random packings. The prediction from computer generated random packing matched the experiments, but both FCC and rhombic packings that are very dense packing produced a larger force on the bottom platen. This suggests that distributed filling through a sieve as used in the experiments has probably led to a packing structure that is random. Further analysis of the microstructure using some fabric descriptors for the particle orientation and void characteristics should provide further insight into the phenomenon.
Figure 7.2 Force on the bottom platen for different particle separations during confined compression of glass beads

Figure 7.3 Force on the bottom platen for different packing structures during confined compression of glass beads
Figures 7.4 and 7.5 show the predicted lateral pressure ratio $K$ and mobilized bulk wall friction coefficient $\mu_{\text{bulk}}$ for the three particle generation schemes used for glass beads. It can be seen that spacings of $1.50d$ and $2.00d$ both produced the same DEM predictions of the average $K$ and $\mu_{\text{bulk}}$. Spacing of $1.01d$ predicted a smaller mobilised bulk wall friction, which is in line with the larger force on the bottom platen (Eqs. 6.1-6.2). The lateral pressure ratio and mobilized bulk wall friction for different packing structures of glass beads are plotted in Figures 7.6 and 7.7. The three packing structures led to different values of $K$ with the rhombic packing producing the smallest $K$ and the random packing producing the largest $K$. However the influence of these packing structures on the value of $\mu_{\text{bulk}}$ is small. Sensitivity to packing structure thus depends on what one attempts to predict.
Figure 7.4 Lateral pressure ratio for different particle separations during confined compression of glass beads

Figure 7.5 Mobilized bulk wall friction coefficient for different particle separations during confined compression of glass beads
Figure 7.6 Lateral pressure ratio for different packing structures during confined compression of glass beads

Figure 7.7 Mobilized bulk wall friction coefficient for different packing structures during confined compression of glass beads
Figure 7.8 shows the force on the bottom platen during confined compression of corn grains for particle generation schemes with different initial particle spacings. All three cases gave reasonable match with the experiments, with the 1.01$d$ case giving the best match. This suggests that corn grains (non-spherical particles) may be less sensitive to particle generation schemes. Figures 7.9 and 7.10 show the lateral pressure ratio and mobilized bulk wall friction coefficient for the three different initial particle spacings. Particle spacing used in generation has some noticeable influence on $K$ value and very small influence on $\mu_{\text{bulk}}$ value predicted. Again for corn, the DEM outcomes are not so sensitive to the choice of particle spacing.

![Figure 7.8](image)
Figure 7.9 Lateral pressure ratio for different particle separations during confined compression of corn grains

Figure 7.10 Mobilized bulk wall friction coefficient for different particle separations during confined compression of corn grains
Figure 7.11 shows the influence of packing structure on the force-displacement responses during rod penetration of glass beads. The generation schemes that gave very dense packing (FCC, Rhombic and 1.01d spacing) all resulted in higher penetration forces than experiments. The amplitudes of force fluctuation also appeared much larger for the denser packings. The random packing and the 1.50d & 2.00d cases all led to a good match with the experiments, again indicating that the glass beads were probably randomly packed in the experiments.

Figure 7.12 shows the force-displacement responses during rod penetration of corn grains for the different particle generation schemes. All three cases of 1.01d, 1.50d and 2.00d gave good match with the test results. Again, corn grains (non-spherical particles) appear to be less sensitive to this factor.
Figure 7.11 Force-displacement responses for different packing structures during rod penetration of glass beads

Figure 7.12 Force-displacement responses for different particle separations during rod penetration of corn grains
7.3 Particle elastic stiffness

Particle stiffness is sometimes reduced in DEM simulations to reduce computational time, since the critical time step is inversely proportional to $\sqrt{G}$ (Eq. 3.36). For some classes of problems, particle stiffness may not have a significant influence on the prediction and may therefore be reduced to gain computational advantage. In this study, the assumed value of shear modulus $G$ was reduced to $0.01G_0$, $0.0001G_0$ to explore sensitivity to $G_0$.

Figures 7.13 (a) and (b) show the force-displacement responses for confined compression of glass beads and corn grains for different shear moduli ($G_0$, $0.01G_0$, $0.0001G_0$). It is expected that the bulk stiffness in confined compression would be directly influenced by the particle stiffness. The relationship between particle stiffness and bulk stiffness can be further deduced from these results (See Section 7.6). Figure 7.14 shows the force transmission onto the bottom platen for these confined compression simulations. Whilst particle stiffness directly influences the bulk stiffness of the system, these results show that it has much less influence on the force transmission onto the boundary surfaces. Especially for corn, reducing stiffness by 100 times produced no noticeable effect on force transmission. For glass beads, reducing particle stiffness did cause a reduction in the force transmitted to the bottom platen: the cause for this is evident from the next figure.

Figure 7.15 shows the mobilized bulk wall friction coefficient versus the height at a top load of 800 N for glass beads and at a top load of 900 N for corn grains. It can be seen that reducing the particle stiffness allows larger displacements under load (consolidation), further mobilising the wall friction. This is particularly true for glass beads that are much stiffer at full stiffness $G$. 

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Figure 7.13 Force-displacement responses for different shear moduli during confined compression
Figure 7.14 Force transmission onto the bottom platen for different shear moduli during confined compression
Figure 7.15 Mobilized bulk wall friction coefficient versus the height for different shear moduli

a) At a top load of 800 N for glass beads

b) At a top load of 900 N for corn grains
The influence of particle stiffness on the force-displacement response during rod penetration of glass beads is shown in Figure 7.16. Reducing particle stiffness appears to have little influence on the average penetration force. However, the magnitude of force fluctuation appears to reduce when particle stiffness is reduced by $10^4$ times. Based on these findings, the shear modulus was reduced by $10^2$ times for all simulations of corn grain rod penetration to reduce the computation time.

![Figure 7.16](image)

**Figure 7.16** Force-displacement responses for different shear moduli during rod penetration of glass beads
7.4 Inter-particle friction

As mentioned in Section 5.3.2, the literature on the measurement of individual inter-particle friction coefficient for irregularly shaped grains is extremely limited. Some limited numerical studies of the influence of inter-particle friction on bulk friction have been reported in the literature (e.g. Walton, 1994). In this study, the values for the inter-particle friction coefficients were assumed to be the same as those for the particle-surface friction coefficients in all the DEM simulations unless otherwise stated. Accordingly, it is important to investigate the validity of the assumption and the influence of inter-particle friction in this study. The reference inter-particle friction $\mu$ for glass beads was taken as 0.244 and $\mu$ was varied between 0.5, 2.0, 4.0 times of the reference value. The reference inter-particle friction for corn grains was 0.335 and simulations with $\mu$ halved and doubled were performed.

Figure 7.17 shows the force transmission onto the bottom platen during confined compression of glass beads and corn grains for different inter-particle friction coefficients. For glass beads, increasing inter-particle friction did not produce a definite trend, with the bottom contact force remaining largely the same. For corn grains, the bottom force increased as the inter-particle friction was increased. This effect for corn grains matches with the observed influence of inter-particle friction on the lateral pressure ratio in the next figure.

The glass beads are also noted to display more sudden unloadings especially for higher inter-particle friction, but these are much less evident for the softer corn grains. The experiments did not show any significant unloading for both materials. This is probably because the experiments were conducted at 1.5 mm/min displacement rate whereas the DEM simulations were performed at 50 mm/min.

Figure 7.18 shows the lateral pressure ratio and mobilized bulk wall friction coefficient calculated from the boundary forces in DEM simulations of confined compression of corn grains. It is not surprising that bulk wall friction $\mu_{\text{bulk}}$ remained relatively unchanged since wall friction coefficient has been kept constant.
throughout. The lateral pressure ratio $K$ increased as the inter-particle friction was decreased. It appears that reducing the inter-particle friction has allowed more of the particle contacts to reach limiting friction, resulting in larger lateral forces and therefore a larger $K$ value. The larger lateral forces gave rise to a large frictional traction being generated on the cylindrical wall, resulting in a smaller force on the bottom platen as reported in the last figure.
Figure 7.17 Force transmission onto the bottom platen for different inter-particle friction coefficients during confined compression
Figure 7.18 Influence of inter-particle friction on silo design parameters for confined compression of corn grains
The influence of inter-particle friction on rod penetration is shown in Figure 7.19. It can be seen that for both corn grains and glass beads halving $\mu$ produced a reduction in the penetration force but doubling $\mu$ did not produce a noticeable increase in the force. Increasing $\mu$ even further appears to produce only a minor effect in the average penetration force. Combining with the observation that particle-boundary friction has no noticeable effect on the rod penetration force (Figure 7.22), it seems that the resistance of a rod penetrating into a granular body comes from the mobilisation of internal friction in the granular assembly adjacent to the rod and not from the surface friction of the rod.

The non-linear effect of inter-particle friction on a bulk response is an important observation that can be seen also in other loading cases and will be discussed further with the angle of repose calculations shown in Figure 7.21.

Figures 7.20 (a) and (b) show the influence of inter-particle friction on the mass flow rate in silo discharge. Inter-particle friction was varied from 0.0244 to 0.9760 for glass beads and from 0.0335 to 1.005 for corn grains. The non-linear effect of inter-particle friction is again evident here. When inter-particle friction increased from 0 to 0.2, the mass flow rate reduced significantly. However, when inter-particle friction increased from say 0.5 to 1.0, mass flow rate did not vary much. This non-linear effect of inter-particle friction on the flow rate is not explicitly stated in the Beverloo formula, so this new finding is a useful refinement on the formula.
Figure 7.19 Force-displacement responses for different inter-particle friction coefficients during rod penetration

a) Glass beads

b) Corn grains
Figure 7.20 Influence of inter-particle friction on mass flow rate
Figure 7.21 shows the effect of inter-particle friction on the angle of repose for corn grains. The results were obtained for the repose angle of the conical pile from the discharge of the cylinder with 0.6D orifice. Again, the non-linear influence of inter-particle friction on bulk friction is observed in the angle of repose. This phenomenon was also reported by Walton (1994), as shown in Figure 7.21. Walton’s results were obtained for uniform 3.78 mm diameter spheres in 12.6 cm diameter rotating drum simulations at rotation rate of 1.571 rad/s. One explanation is that when the inter-particle friction is small, inter-particle friction is more easily fully mobilised, so the majority of the contacts are at limiting friction condition. For such scenario, one would expect a direct dependency of bulk friction on inter-particle friction. However as inter-particle friction becomes larger, the majority of the particle contacts may not reach the limiting friction condition, resulting in weaker dependency of the bulk friction on particle friction. The actual phenomenon may be more complex than this simple description. A deeper exploration of the characteristics of the inter-particle contact forces from these DEM simulations should provide further insight, but this is beyond the scope of this study due to time constraint.

![Graph showing the effect of inter-particle friction on the angle of repose for corn grains.](image)

**Figure 7.21** Angle of repose versus inter-particle friction coefficient for corn grains
7.5 Particle-boundary friction

The influence of particle-boundary friction on rod penetration is shown in Figure 7.22. The particle-rod friction coefficient was varied between 0.5, 1.0, 4.0 times of the reference value of 0.244 for glass beads and between 0.5, 1.0, 2.0 times of the reference value of 0.335 for corn grains. It can be seen that the particle-rod friction has no noticeable effect on the force-displacement response during rod penetration for both materials.
Figure 7.22 Force-displacement responses for different particle-rod friction coefficients during rod penetration
7.6 Relation between particle stiffness and bulk stiffness

The relationship between particle stiffness and bulk stiffness can be deduced from the force-displacement responses in confined compression for different particle shear moduli, as shown in Figure 7.13. In this first approximation, the shear force on the cylindrical wall is assumed to be negligible. The average vertical stress \( \sigma_z \) is determined from the average of the top and bottom forces and the radial stress \( \sigma_r \) can be calculated from the normal force on the wall. The isotropic elastic stress-strain relations in the cylindrical coordinate system are given by

\[
e_r = \frac{1}{E_{\text{bulk}}} \left[ \sigma_r - \nu_{\text{bulk}} (\sigma_\theta + \sigma_z) \right]
\]

\[
e_\theta = \frac{1}{E_{\text{bulk}}} \left[ \sigma_\theta - \nu_{\text{bulk}} (\sigma_r + \sigma_z) \right]
\]

\[
e_z = \frac{1}{E_{\text{bulk}}} \left[ \sigma_z - \nu_{\text{bulk}} (\sigma_r + \sigma_\theta) \right]
\]

In Eqs. (7.1-7.3): \( E_{\text{bulk}} \) and \( \nu_{\text{bulk}} \) are the bulk Young's modulus and Poisson's ratio of the granular solid respectively; \( \epsilon_r \), \( \epsilon_\theta \) and \( \epsilon_z \) are the radial strain, hoop strain and vertical strain respectively; \( \sigma_\theta \) is the hoop stress of the granular solid.

Assuming rigid confinement so that the radial strain \( \epsilon_r \) and hoop strain \( \epsilon_\theta \) are zero, the bulk Young's modulus \( E_{\text{bulk}} \) can be written as Eq. (7.4) by rearranging Eqs. (7.1-7.3).

\[
E_{\text{bulk}} = \frac{(1 + \nu_{\text{bulk}})(1 - 2\nu_{\text{bulk}})}{(1 - \nu_{\text{bulk}})} \frac{\sigma_r}{\epsilon_z}
\]

The bulk tangent Young's modulus \( E_{\text{bulk}} \) at a given state of loading can be expressed in incremental form as
Eq. (7.5) can be used to determine the bulk tangent Young’s modulus $E_{\text{bulk}}$ at different vertical stresses from the non-linear force-displacement responses for various particle stiffness values. For example, consider the confined compression of glass beads with particle stiffness values of $G_0$, $0.1G_0$, $0.01G_0$, $0.001G_0$ and $0.0001G_0$, as shown in Figure 7.23. The reference value of particle shear modulus $G_0$ was 17 GPa, as measured for the glass beads. Using Eq. (7.5) and assuming Poisson’s ratio $\nu_{\text{bulk}} = 0.25$, the relationship between the bulk tangent Young’s modulus and particle stiffness ratio at different vertical stresses (i.e. 300, 500 and 700 kPa) can be calculated and shown in Figure 7.24. Both the bulk tangent Young’s modulus and particle stiffness ratio are based on log scales and generally show a linear relationship. This indicates that both quantities have a power law relationship of the form $E_{\text{bulk}} / E_{\text{bulk},o} = k(G / G_0)^n$. The reference value of bulk tangent Young’s modulus $E_{\text{bulk},o}$ was 26 MPa, calculated for the reference value $G_0$ at vertical stress of 300 kPa. Using linear regression, the best fit values for $k$ and $n$ can be determined and are given in Table 7.3 for various vertical stresses. In short, this simple analysis shows that for confined compression, the bulk stiffness is approximately proportional to the square root of the particle modulus ratio. The results can be replotted to explore the bulk stiffness variation as a function of vertical stress. Figure 7.25 show the relationship between the bulk tangent Young’s modulus ratio $E_{\text{bulk}} / E_{\text{bulk},o}$ and vertical stress.

\[
E_{\text{bulk}} = \frac{(1 + \nu_{\text{bulk}})(1 - 2\nu_{\text{bulk}}) \Delta \sigma_z}{(1 - \nu_{\text{bulk}}) \Delta \varepsilon_z}
\] (7.5)

<table>
<thead>
<tr>
<th>Vertical stress (kPa)</th>
<th>$k$</th>
<th>$n$</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>0.92</td>
<td>0.49</td>
</tr>
<tr>
<td>500</td>
<td>1.49</td>
<td>0.52</td>
</tr>
<tr>
<td>700</td>
<td>2.14</td>
<td>0.54</td>
</tr>
</tbody>
</table>
Figure 7.23 Force-displacement responses for different shear moduli during confined compression of glass beads

Figure 7.24 Bulk tangent Young’s modulus versus particle stiffness ratio
7.7 Summary

The influence of DEM input parameters has been explored extensively to study the sensitivity of single particle (micro) properties on the bulk (macro) behaviour of a dense granular system. The DEM input parameters studied include the particle generation scheme (initial packing structure), particle elastic stiffness, inter-particle friction and particle-boundary friction. This parametric study has resulted in many useful observations with significant implications for the relative importance of the DEM input parameters. The chief conclusions are:

1. Initial particle packing condition has been shown to affect the DEM outcomes, so consideration must be given to how the particles are generated to model the actual initial packing structure. Sensitivity to initial packing structure varies depending on the parameter of interest. Uniform spheres can sometimes get into crystalline formation and additional simulations by setting up rhombic and FCC packings of spheres show how uniform spheres can get into packing structure that gives a significantly different bulk response. For corn grains (non-spherical
particles), as long as some settling down is permitted, DEM results were found to be not so sensitive to the particle spacing used in particle generation.

2. Whilst particle stiffness directly influences the bulk stiffness of the system during confined compression, it has a much smaller influence on the boundary contact forces. Reducing stiffness up to $10^4$ times produced no effect on the average rod penetration force, whilst providing a huge computational advantage.

3. The non-linear influence of inter-particle friction on bulk friction has been established, providing a basis for explaining several phenomena observed.

4. Rod penetration force does not depend significantly on rod friction for up to 60 mm penetration. The resistance of a rod penetrating into a granular body appears to come from the mobilisation of internal friction in the granular assembly adjacent to the rod and not from the surface friction of the rod.

5. A power law relationship between particle stiffness and bulk stiffness has been derived from the DEM results for confined compression of glass beads.
Chapter 8

A study of the influence of gravity

8.1 Introduction

For any significant exploration of the Moon and Mars, most mission scenarios require In Situ Resource Utilization (ISRU). A typical example is to make propellant for the return journey from Mars to Earth using carbon and oxygen from the Martian atmosphere and hydrogen from ice excavated beneath the Martian surface. Most of the relevant in-situ resources of the Moon and Mars are found in the regolith i.e. the loose layer of sand and rocks covering the surface. Developing technology for these geomaterials is therefore of paramount importance to the extraterrestrial exploration. For this purpose, the properties and mechanics of the extraterrestrial regoliths have to be well understood in order to predict the behaviours of granular geomaterials in the lunar and Martian environments, which will form the basis to develop methodologies for dealing with the ISRU processes. This chapter describes a numerical study to explore the influence of gravity on the loading cases investigated in this thesis. It was conducted in response to the NASA’s call for granular mechanics research on regolith and will be presented in the NASA 2nd Workshop on Granular Materials in a Lunar and Martian Exploration to be held in conjunction with the ASCE Earth and Space 2006 Conference in Houston in March 2006.
Understanding and predicting how the regoliths will respond is clearly a primary objective in preparation for the lunar and Martian exploration. The discrete element method (DEM) is by now a well-established method for modelling granular assemblies. Two advantages of this approach are that complex stress-strain behaviour is replaced by much simpler particle behaviour, and that localised regions, such as fractures and rupture zones, develop naturally as part of the simulation (Cundall, 2001). Although the application of particle methods to large-scale problems is currently difficult or impossible because of high computational demands, Cundall (2001) clearly predicted that such applications should be feasible within ten years and certainly within 20 years (when computing power becomes sufficient to support such simulations). DEM has been shown to be a very promising tool for many terrestrial applications and there is every reason to believe that it can become an effective numerical tool for lunar and Martian applications when particle scale behaviour dominates.

However, as mentioned in Chapter 1, most DEM simulation results were often not validated or compared with experimental results. Furthermore, the input parameters used in the DEM simulations were often simply given without any explanation and seldom measured in laboratory tests, so influence of the input parameters on the prediction outcomes can be rather obscure. Therefore, validating if a DEM code can produce satisfactory predictions is a necessary precursor.

A series of DEM computations under the Moon’s gravity was performed to simulate the experiments studied in this thesis, namely filling a cylinder, vertical confined compression, discharging and rod penetration into the granular medium. Similar loading and flow conditions are likely to be encountered in the stress and deformation regimes that the regoliths will be subjected to in the lunar exploration activities including the ISRU processes. By linking into the extensive study under terrestrial gravity presented in early chapters which include a detailed comparison between experiments and DEM computations on both spherical (glass beads) and non-spherical (corn grains) particles, this study of the influence of gravity provides a useful contribution to the research of regolith mechanics.
8.2 Gravity effect

The gravity on the Moon is one-sixth that on the Earth. The following cases were simulated using the reduced lunar gravity and compared with the results with Earth's gravity: (1) confined compression of glass beads; (2) rod penetration of glass beads; and (3) silo discharge of corn grains.

Figure 8.1 shows the force on the bottom platen under different gravities (g and g/6, \( g = 9.81 \text{m/sec} \)) during confined compression of glass beads. It can be seen that gravity has no noticeable effect on the force transmission in confined compression, which is not surprising.

Figure 8.2 shows the force-displacement responses under different gravities during rod penetration of glass beads. The average trends obtained by the least square method are also indicated. The gradients are 0.1456 N/mm and 0.0234 N/mm for the gravities g and g/6 respectively. The gradient for Earth's gravity is thus almost six times that for the Moon's gravity, indicating that penetration force is linearly proportional to the gravitational acceleration.

Figure 8.3 shows the mass flow rates under different gravities (g, g/6 and g/12) during discharging of corn grains from the cylinder with 0.6D orifice. It can be seen that the mass flow rate decreases as the gravity decreases, with the corresponding increase in the discharge duration. Table 8.1 shows the mass flow rates calculated from the DEM simulations under different gravities. The mass flow rates predicted by Beverloo formula (Eq. 6.6) are also shown in Table 8.1. The predicted mass flow rates match well with Beverloo formula. The discharge rate is thus proportional to the square root of the gravitational acceleration.

Table 8.1 also shows the angle of repose under different gravities. It can be seen that the angle of repose increases with the decrease of the gravity.
Table 8.1 Mass flow rate and angle of repose under different gravities for corn grain discharge

<table>
<thead>
<tr>
<th>Gravity</th>
<th>Mass flow rate (kg/sec) from Beverloo formula</th>
<th>Mass flow rate (kg/sec) from DEM</th>
<th>Angle of repose (degree) from DEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>g (on earth)</td>
<td>3.132</td>
<td>3.185</td>
<td>28.0</td>
</tr>
<tr>
<td>g/6 (on moon)</td>
<td>1.272</td>
<td>1.262</td>
<td>31.3</td>
</tr>
<tr>
<td>g/12</td>
<td>0.908</td>
<td>0.901</td>
<td>32.8</td>
</tr>
</tbody>
</table>

Figure 8.1 Force on the bottom platen under different gravities during confined compression of glass beads
Figure 8.2 Force-displacement responses under different gravities during rod penetration of glass beads

Figure 8.3 Mass flow rate under different gravities during discharging of corn grains
8.3 Summary

The gravity influence on the bulk responses of a dense granular medium has been explored in this chapter. The chief conclusions are as follows:

1. The gravity has no noticeable effect on the force transmission in the confined compression case.
2. The slope of the force-displacement response in rod penetration is proportional to the gravity.
3. The mass flow rate in silo discharge is proportional to the square root of the gravity, as interpreted in Beverloo formula (Beverloo et al., 1961).

These are in agreement with the expectations.
Chapter 9

Linking of DEM with FEA to evaluate boundary stresses

9.1 Introduction

To evaluate the effect of the particle forces acting on a deformable body, it is sensible to link the DEM simulation outcomes to a finite element package. This chapter describes the implementation with Abaqus FEA package. The mathematical formulation to convert the DEM boundary contact forces to the nodal forces and moments in a triangular mesh element has been derived based on the shape function concept. A Fortran program has been coded for this purpose and validated by performing a verification example with ABAQUS. After ensuring that the program was coded correctly, the DEM results from the confined compression simulation were extracted and processed into an ABAQUS input file. A finite element analysis was carried out to calculate the stress distribution in the cylinder using a linear shell analysis.

9.2 Basic concepts

The DEM output in both EDEM and PFC gives the resultant force and moment (in the global coordinate system) acting at the centroid of each triangular boundary element. The first task is to convert the resultant contact force and moment for each
element to the equivalent nodal forces in the global coordinate system. This was
done using the shape functions for 3-node plate element. Once the equivalent nodal
forces for each triangular element are found, the stresses in the deformable body can
be determined by conducting the FEA calculation using any FEA software
(ABAQUS, ANSYS, etc).

\section*{9.3 Mathematical formulation}

Consider a triangular element and the contact forces resulting from particles are
applied at the centroid of the triangular element. Set up a local coordinate system (x, y, z) at the centroid P, as shown in Figure 9.1. Plane x-y is coincident with the plane
of the triangular element. Let \( \vec{u}_{ij} \) denote the unit vector along the line joining point i
and point j and \( \vec{u}_{ik} \) the unit vector along the line joining point i and point k. The
normal unit vector, \( \vec{n} \), of the triangular element is determined by

\[ \vec{n} = \frac{\vec{u}_{ij} \times \vec{u}_{ik}}{|\vec{u}_{ij} \times \vec{u}_{ik}|} \tag{9.1} \]

Let x direction be coincident with \( \vec{u}_{ij} \) and then the three unit vectors \( \vec{u}_x \), \( \vec{u}_y \) and \( \vec{u}_z \)
of the local coordinate system can be expressed as

\[ \vec{u}_x = \vec{u}_{ij} \tag{9.2} \]

\[ \vec{u}_z = \vec{n} \tag{9.3} \]

\[ \vec{u}_y = \vec{n} \times \vec{u}_x \tag{9.4} \]

The relationship between the local coordinate system (x, y, z) and the global
coordinate system (X, Y, Z) can be expressed as

\[ \{x, y, z\}^T = [T_{trans,1}]\{X, Y, Z\}^T \tag{9.5} \]
where \( [T_{\text{trans,1}}] \) is a 3×3 transformation matrix and is given by

\[
[T_{\text{trans,1}}] = \begin{bmatrix} \bar{u}_x & \bar{u}_y & \bar{u}_z \end{bmatrix} \begin{bmatrix} u_x & u_y & u_z \end{bmatrix}^T
\]  

(9.6)

Now consider that each node has 6 degrees of freedom (three displacements, \( u_x, u_y, u_z \), and three rotations, \( \theta_x, \theta_y, \theta_z \)), but \( \theta_z \) can be assumed to be negligible. The displacement field \( \{U\}_{6\times1} \) can be related to the nodal displacements \( \{A\}_{18\times1} \) via the shape function \( [N]_{6\times8} \) as

\[
\{U\}_{6\times1} = [N]_{6\times8} \{A\}_{18\times1}
\]

(9.7)

where \( [N]_{6\times8} \) is the shape function matrix for a 3-node plate element. It has a very complex form (Specht, 1988; Zienkiewicz and Taylor, 2000) and is outlined in Appendix E. The matrices \( \{U\}_{6\times1} \) and \( \{A\}_{18\times1} \) are expressed as

\[
\{U\}^T = \{u_x, u_y, u_z, \theta_x, \theta_y, \theta_z\}
\]

(9.8)

\[
\{A\}^T = \{u_{x1}, u_{y1}, u_{z1}, \theta_{x1}, \theta_{y1}, \theta_{z1}, \ldots, u_{xk}, u_{yk}, u_{zk}, \theta_{xk}, \theta_{yk}, \theta_{zk}\}
\]

(9.9)
External virtual work induced by contact forces is given by

$$\delta W = \{\delta U_p\}^T \times 6 \{\vec{F}_{\text{con}, P}\}_{6 \times 6} \tag{9.10}$$

where $$\{\vec{F}_{\text{con}, P}\}$$ is the contact force vector applied at the centroid in the local coordinate system and subscript P refers to the centroid of the triangular element. Substituting Eq. (9.7) into Eq. (9.10) gives Eq. (9.11).

$$\delta W = \{\delta A\}^T \times 6 \times [N_p]_{18 \times 6} \{\vec{F}_{\text{con}, P}\}_{6 \times 6} \tag{9.11}$$

From Eq. (9.11), the equivalent nodal forces in the local coordinate system can be expressed as

$$\{\vec{F}_{\text{con, nodal}}\}_{18 \times 1} = [N_p]_{18 \times 6} \{\vec{F}_{\text{con, P}}\}_{6 \times 6} \tag{9.12}$$

Using the coordinate transformation, the contact forces in the local coordinate system can be related to the contact forces in the global coordinate system as

$$\{\vec{F}_{\text{con, P}}\}_{6 \times 1} = [T_{\text{trans}, 2}]_{6 \times 6} \{\vec{F}_{\text{con, P}}\}_{6 \times 6} \tag{9.13}$$

where $$[T_{\text{trans}, 2}]$$ is a $$6 \times 6$$ transformation matrix and is given by

$$[T_{\text{trans}, 2}] = \begin{bmatrix} [T_{\text{trans}, 1}] & [0] \\ [0] & [T_{\text{trans}, 1}] \end{bmatrix} \tag{9.14}$$

Similarly, the equivalent nodal forces in the global coordinate system can be related to the equivalent nodal forces in the local coordinate system as

$$\{F_{\text{con, nodal}}\}_{18 \times 1} = [T_{\text{trans}, 3}]_{18 \times 18} \{F_{\text{con, nodal}}\}_{18 \times 1} \tag{9.15}$$

where $$[T_{\text{trans}, 3}]$$ is a $$18 \times 18$$ transformation matrix and is given by
Substituting Eqs. (9.12-9.13) into Eq. (9.15) leads to Eq. (9.17). This equation relates the equivalent nodal forces in the global coordinate system to the contact forces in the global coordinate system.

\[
\begin{bmatrix}
T_{\text{trans},2} & 0 & 0 \\
0 & T_{\text{trans},2} & 0 \\
0 & 0 & T_{\text{trans},2}
\end{bmatrix}
\]

(9.16)

\[
\{F_{\text{con,nodal}}\}_\text{1x6} = \left[T_{\text{trans},3}\right]_{1\times18}^{\text{T}} \left[N_p\right]_{18\times6}^{\text{T}} \left[T_{\text{trans},2}\right]_{6\times6} \{F_{\text{con,p}}\}_\text{6x1}
\]

(9.17)

### 9.4 Verification example

A verification example for a triangular thin plate supported by three vertex nodes was devised to verify the computation of the equivalent nodal forces. This triangular plate has a thickness of 10 mm and side lengths of 5, 10 and 12 m and the material properties are as follows: Young’s modulus = 209 GPa; Poisson’s ratio = 0.3. Consider the concentrated forces and moments acting on the plate. Two approaches are used: (1) introduce additional nodes so that the points of applied forces and moments are also the finite element nodes and directly use ABAQUS to calculate the reaction forces; (2) using the Fortran program written, convert the applied forces and moments into the nodal forces and moments in the same finite element mesh (without the additional nodes) and then use ABAQUS to calculate the reaction forces. Methods (1) and (2) should give exactly the same outcomes. An ABAQUS element type STRI3 (3-node triangular facet thin shell) was used to represent the triangular thin plate and a linear analysis was performed in this example.

Figures 9.2 and 9.3 show finite element meshes and node numbering of a triangular plate for Method (1) and Method (2), respectively. The vertices of the triangular plate denoted by node number 2, 3 and 4 are fixed in the translational and rotational degrees of freedom. Method (1) used 697 nodes and 1272 elements, whereas Method (2) used 694 nodes and 1266 elements. The two meshes are identical except the magnified areas, as shown in Figures 9.2 and 9.3. The concentrated forces and
moments are applied at the nodes with node number 10000, 20000 and 30000. These nodes are the centroids of the triangles consisting of node number: 1, 5, 243; 1, 243, 76; 1, 76, 420, respectively (Figure 9.2).

Consider three loading cases as shown in Table 9.1. Tables 9.2-9.4 show the comparisons for the reaction forces between Method (1) and Method (2) in the Loading Cases I, II and III respectively. It can be seen that for Cases I and II where the concentrated torque (i.e. $M_\tau$) is absent, the results from Method (2) are the same as those from Method (1). In Case III, the normal force ($F_z$), bending moments ($M_x$ and $M_y$) are the same for both methods, but the in-plane forces ($F_x$ and $F_y$) are different due to the presence of the concentrated torque ($M_\tau$). This is attributed to the fact that the degree of freedom for torsion (i.e. $\theta_\tau$) is assumed to be negligible in the mathematical formulation. Thus, this formulation does not apply to the cases where the particle loading imparts a significant $M_\tau$ torque component.

The Fortran code used to convert the contact forces at the centroid of the triangular element in the global coordinate system to the equivalent nodal forces in the global coordinate system has been developed and validated by this example. It can be seen that the program is coded correctly.

<table>
<thead>
<tr>
<th>Loading condition</th>
<th>Node No.</th>
<th>$F_x$ (N)</th>
<th>$F_y$ (N)</th>
<th>$F_z$ (N)</th>
<th>$M_x$ (N-m)</th>
<th>$M_y$ (N-m)</th>
<th>$M_z$ (N-m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>10000</td>
<td>0</td>
<td>0</td>
<td>300</td>
<td>300</td>
<td>300</td>
<td>0</td>
</tr>
<tr>
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<td>20000</td>
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<td>0</td>
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<tr>
<td></td>
<td>30000</td>
<td>0</td>
<td>0</td>
<td>500</td>
<td>-500</td>
<td>-500</td>
<td>0</td>
</tr>
<tr>
<td>II</td>
<td>10000</td>
<td>100</td>
<td>100</td>
<td>300</td>
<td>300</td>
<td>300</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>20000</td>
<td>200</td>
<td>200</td>
<td>600</td>
<td>600</td>
<td>600</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>30000</td>
<td>300</td>
<td>300</td>
<td>900</td>
<td>900</td>
<td>900</td>
<td>0</td>
</tr>
<tr>
<td>III</td>
<td>10000</td>
<td>300</td>
<td>300</td>
<td>300</td>
<td>300</td>
<td>300</td>
<td>300</td>
</tr>
<tr>
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<td>20000</td>
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<td>-400</td>
<td>-400</td>
<td>-400</td>
<td>-400</td>
<td>-400</td>
</tr>
<tr>
<td></td>
<td>30000</td>
<td>500</td>
<td>500</td>
<td>500</td>
<td>-500</td>
<td>-500</td>
<td>-500</td>
</tr>
</tbody>
</table>
Table 9.2 Comparison between ABAQUS and proposed method in Loading Case I

<table>
<thead>
<tr>
<th>Method</th>
<th>Node No.</th>
<th>( F_x ) (N)</th>
<th>( F_y ) (N)</th>
<th>( F_z ) (N)</th>
<th>( M_x ) (N-m)</th>
<th>( M_y ) (N-m)</th>
<th>( M_z ) (N-m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABAQUS</td>
<td>2</td>
<td>0.0</td>
<td>0.0</td>
<td>-276.8</td>
<td>122.7</td>
<td>-200.5</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>0.0</td>
<td>0.0</td>
<td>-72.0</td>
<td>234.7</td>
<td>22.2</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>0.0</td>
<td>0.0</td>
<td>-51.3</td>
<td>21.2</td>
<td>78.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Proposed method</td>
<td>2</td>
<td>0.0</td>
<td>0.0</td>
<td>-276.8</td>
<td>122.8</td>
<td>-200.5</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>0.0</td>
<td>0.0</td>
<td>-72.0</td>
<td>234.6</td>
<td>22.2</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
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<td>0.0</td>
<td>-51.3</td>
<td>21.2</td>
<td>78.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

Table 9.3 Comparison between ABAQUS and proposed method in Loading Case II

<table>
<thead>
<tr>
<th>Method</th>
<th>Node No.</th>
<th>( F_x ) (N)</th>
<th>( F_y ) (N)</th>
<th>( F_z ) (N)</th>
<th>( M_x ) (N-m)</th>
<th>( M_y ) (N-m)</th>
<th>( M_z ) (N-m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABAQUS</td>
<td>2</td>
<td>-329.5</td>
<td>-20.5</td>
<td>-16.4</td>
<td>191.8</td>
<td>-143.6</td>
<td>1.0E-02</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>-107.9</td>
<td>-484.6</td>
<td>-1618.0</td>
<td>980.9</td>
<td>-335.3</td>
<td>-9.7E-03</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>-162.6</td>
<td>-94.9</td>
<td>-165.3</td>
<td>-82.8</td>
<td>145.3</td>
<td>2.5E-03</td>
</tr>
<tr>
<td>Proposed method</td>
<td>2</td>
<td>-329.5</td>
<td>-20.5</td>
<td>-16.4</td>
<td>191.8</td>
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<tr>
<td></td>
<td>3</td>
<td>-107.9</td>
<td>-484.6</td>
<td>-1618.0</td>
<td>981.0</td>
<td>-335.3</td>
<td>-9.7E-03</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>-162.6</td>
<td>-94.9</td>
<td>-165.3</td>
<td>-82.8</td>
<td>145.3</td>
<td>2.5E-03</td>
</tr>
</tbody>
</table>

Table 9.4 Comparison between ABAQUS and proposed method in Loading Case III

<table>
<thead>
<tr>
<th>Method</th>
<th>Node No.</th>
<th>( F_x ) (N)</th>
<th>( F_y ) (N)</th>
<th>( F_z ) (N)</th>
<th>( M_x ) (N-m)</th>
<th>( M_y ) (N-m)</th>
<th>( M_z ) (N-m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABAQUS</td>
<td>2</td>
<td>-135.9</td>
<td>29.2</td>
<td>-276.8</td>
<td>122.7</td>
<td>-200.5</td>
<td>2.3E-04</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>-183.5</td>
<td>-368.2</td>
<td>-72.0</td>
<td>234.7</td>
<td>22.2</td>
<td>-1.1E-02</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>-80.7</td>
<td>-60.9</td>
<td>-51.3</td>
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Figure 9.2 Finite element mesh and node numbering for triangular plate in Method (1)
Figure 9.3 Finite element mesh and node numbering for triangular plate in Method (2)
9.5 Numerical example for confined compression

The confined compression of glass beads in the cylinder was chosen as an example application. ABAQUS element type STRI3 (3-node triangular facet thin shell) was used to represent the cylindrical shell. The thin walled cylinder (diameter = 145 mm, length = 300 mm, thickness = 3.33 mm) is made from acrylic (Young’s modulus = 2.9 GPa, Poisson’s ratio = 0.35). The number of nodes for cylindrical wall is 272 and the number of finite elements is 512. The nodes at the bottom are fixed in the translational and rotational degrees. A linear analysis was performed in this example.

Figures 9.4-9.7 show the FEA predicted Mises stress distributions in the cylinder at the applied top load of 132, 295, 680 and 932N respectively. It can be seen that as vertical loading increases, the Mises stress increases overall with a larger increase near the top, as expected. This simple example was done to demonstrate the methodology and NOT to produce an accurate FEA prediction of the stresses in the cylinder. The same mesh for the boundary elements in the DEM simulation was used for the FEA analysis. The high stresses all occur at the central node of a cross, at the middle of adjacent flat plate elements. This is caused by the flat plate finite elements which bend instead of a curved wall which stretches. With the linking from the DEM results, the rather coarse triangular element mesh from DEM was used for the FEA analysis. Refining the mesh may improve the FEA prediction but may not remove the stress concentration altogether. A typical ABAQUS input file can be found in Appendix E.
Figure 9.4 FEA Mises stress distribution at a top load of 132N in confined compression

Figure 9.5 FEA Mises stress distribution at a top load of 295N in confined compression
Figure 9.6 FEA Mises stress distribution at a top load of 680N in confined compression

Figure 9.7 FEA Mises stress distribution at a top load of 932N in confined compression
9.6 Summary

A methodology to link the DEM simulation results with the finite element method has been presented in this chapter. The mathematical formulation to convert the DEM boundary contact forces to the nodal forces and moments in a triangular mesh element has been derived based on the shape function concept and implemented in a Fortran program. A verification example showed that this program was coded correctly and a numerical example modelling the confined compression of glass beads was then illustrated.
Chapter 10

General conclusions and recommendations

10.1 General conclusions

In this study, DEM simulations have been extensively used to model spherical (glass beads) and non-spherical (corn grains) grains under a variety of loading scenarios. The main achievements are:

1. Physical calibration experiments of filling, compression, penetration and discharging have been developed and conducted;
2. Methodologies and experimental apparatuses to measure the main particle parameters (Young’s modulus, friction coefficient and restitution coefficient) for DEM models have been established;
3. Measurements of the mechanical and geometric properties for samples of corn, wheat and glass beads have been conducted. This provides a database of measurements that can be used for simulations of grain dynamics;
4. A set of eight benchmark tests have been performed to validate the DEM codes and to enhance the understanding of fundamental impact phenomena;
5. A large number of DEM simulations have been conducted and comparison between DEM simulations and experiments has been made.
6. The influence of DEM input parameters has been explored extensively, providing a useful insight into the effects of single particle (micro) properties on the bulk (macro) behaviour;
7. The influence of the gravitational acceleration on the bulk responses of a granular solid has been examined;
8. A methodology to link DEM with FEA has been developed. This can be used to determine the stresses in the contacting body resulting from particle forces.

A summary by chapter of the key conclusions from this study is as follows:

Chapter 3
The Rayleigh wave concept and the natural frequency concept for calculating the critical time step both gave comparable outcomes. The study of O’Sullivan and Bray (2004c) showed that the critical time step is a function of the packing condition and coordination number, and for 3D uniform-sized spheres, it should be less than $0.22 \sqrt{m/K}$. It is suggested that this provides a sound reference value for the computational time step in DEM simulations and a multiplier of 20% is appropriate.

Chapter 4
All benchmark tests showed good to excellent match, providing quantitative checks for the DEM codes. The analytical solutions provide an excellent insight into particle impact mechanics. The DEM computations also provide further information on some aspects in the sticking regime for oblique impact, where the analytical solutions can only provide upper bound values.

Chapter 5
The Young’s modulus for individual corn grains was evaluated using two methods: the ASAE indenter method and the proposed rigid platen compression method. The test results from the two methods were comparable. This ASAE indenter method was found to be not suitable for grains that are not sufficiently flat at the region of contact. The proposed method together with the radii of curvature measured using a 3D laser scanner has been shown to be stable during the single particle compression
test and can be applied to any irregularly shaped agricultural grains. A sliding test apparatus was devised to measure the static particle-surface friction coefficients. This sliding friction test has been shown to be stable and reproducible. A drop test apparatus has been built to determine the particle-surface restitution coefficient. A new methodology to determine the restitution coefficient for irregularly shaped particles has been presented.

Chapter 6

Comparison between DEM simulations and physical experiments has been made. The majority showed good to excellent match, providing a quantitative validation for the DEM simulations of the problems studied.

More specifically:

For glass beads: DEM gave good agreement with experiments for silo filling (normal wall pressure distribution), confined compression (normal wall pressure distribution, load transfer to boundary surfaces), rod penetration (force-displacement response), and silo discharge (mass flow rate), but under-predicted bulk wall friction $\mu_{\text{bulk}}$ and over-predicted lateral pressure ratio $K$.

For corn grains: the study shows that 4-sphere representation together with the measured corn properties produced good to excellent match with experiments for silo filling (normal wall pressure distribution), confined compression (normal wall pressure distribution, load transfer to boundary surfaces, and bulk design parameters $K$ and $\mu_{\text{bulk}}$), rod penetration (force-displacement response), and silo discharge (mass flow rate and angle of repose). This provides solid verification that DEM is capable of producing quantitative predictions. The findings suggest that very accurate representation of the non-spherical particle shape may not be necessary to produce satisfactory predictions and capturing the key linear dimensions of a particle may be adequate, at least for the load cases studied.
The two main DEM simulations that produced larger discrepancies with experiments are filling density (~8% lower for glass beads and ~17% lower for corn grains) and loading stiffness (stiffer response). Plausible explanations for these were given.

Chapter 7

The study of the influence of DEM input parameters on the bulk response has resulted in many useful observations, with significant implications on the relative importance of the DEM input parameters. The chief conclusions are:

1. Initial particle packing condition has been shown to affect the DEM outcomes, so consideration must be given to how the particles are generated to model the actual initial packing structure. Sensitivity to initial packing structure varies depending on the parameter of interest. For corn grains, DEM results were found to be not so sensitive to the particle spacing used in particle generation.

2. Whilst particle stiffness directly influences the bulk stiffness of the system during confined compression, it has a much smaller influence on the boundary contact forces. Reducing stiffness up to 10000 times produced no noticeable effect on the average rod penetration force, whilst providing a huge computational advantage.

3. The non-linear influence of inter-particle friction on bulk friction has been established, providing a basis for explaining several phenomena observed.

4. Rod penetration force does not depend significantly on rod friction for up to 60 mm penetration. The resistance of a rod penetrating into a granular body appears to come from the mobilisation of internal friction in the granular assembly adjacent to the rod and not from the surface friction of the rod.

5. A simple approach for determining the relationship between particle stiffness and bulk stiffness has been proposed. Both the bulk Young's modulus and particle stiffness ratio have a power law relationship.
Chapter 8

The influence of gravity on the bulk responses of a dense granular medium has been examined for several load cases. The magnitude of the gravitational acceleration $g$ was found to have no noticeable effect on the force transmission in the confined compression. The gradient of the force-displacement response in rod penetration was proportional to $g$ and the mass flow rate in silo discharge was proportional to the square root of $g$. These are in agreement with the expectations.

Chapter 9

A methodology to link the DEM simulation results with the finite element method has been proposed and implemented in a Fortran program. A verification example shows that this program was coded correctly.

10.2 Recommendations for further research

Some potential areas for follow-on research are outlined below.

1. The research has produced a significant body of unique scientific data which can be exploited for more in-depth analysis of the micro and macro features of a dense granular system. The bulk behaviour of the granular material is highly related to the fabric of the granular assembly. The important fabric of the granular medium include the orientation of the elongated particles (the long axis of the particle), distribution of the branch vectors (the vector from one particle centre to that of the contacted neighbour), length of the branch vectors, distribution of contact normal, local voids and coordination number (Ng, 1999; Woodcock, 1977). Further analysis of the microstructure using these fabric descriptors should provide further insight into the behaviour of a granular assembly.

2. Since contact forces propagate through the granular assembly to transmit to the boundary surfaces, the development of the force chains and the internal states of stress and strain within the assembly is important and should to be investigated.
3. Further investigation to confirm whether capturing particle shape using only a limited number of spheres to match the linear dimensions of the particle is sufficient to produce satisfactory predictions.

4. Natural particle size variation exists in the physical experiments. The influence of particle size variation should be further investigated, especially to verify if it is the main reason for the discrepancy in the filling density.

5. The linear or non-linear elastic spring-dashpot contact model widely used in DEM may not be particularly suited for the relatively soft agricultural grains. Engineering predictions that depend on contact energy dissipation or contact stiffness under significant loading will require a better contact model. A DEM contact model for softer agricultural grains can be developed for such purposes.

6. The study of the influence of a subset of the DEM input parameters in this thesis has highlighted the relative importance of these parameters and the complexity involved. It is important that the significance of each parameter is explored to understand its influence in relatively simple loading actions before much more complex loading scenarios are attempted. Further studies are clearly warranted. For example, the effect of the restitution coefficient was not explored in this thesis because it was deemed to be less important for quasi-static situations in this thesis, but for predominantly flowing problems, it should be explored further.

7. Density scaling method to reduce the computational time associated with DEM simulations for quasi-static problems (Thornton and Antony, 2000; O’Sullivan et al., 2004b) is worthy of further study. DEM applications to large-scale problems are currently difficult or impossible due to extensive computer resource requirement, so computational strategies need to be developed for this purpose.
References


Appendix A

Measurements of the physical and mechanical properties for different type of grains

A.1 Physical properties

The measurements of the physical properties for different type grains are listed below (summarised in Section 5.2).

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<th>CornB Mass (g)</th>
<th>CornC Mass (g)</th>
<th>CornD Mass (g)</th>
<th>CornE Mass (g)</th>
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Table A.1 Mass for six types of corn grains
Table A.2 Linear dimensions for ComA corn grains

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Table A.3 Linear dimensions for ComB corn grains

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Table A.4 Linear dimensions for ComC corn grains

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### Table A.6 Linear dimensions for CornE corn grains

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### Table A.7 Linear dimensions for CornF corn grains

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Table A.12 Dense bulk densities for six types of corn grains

<table>
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<th>Corn type</th>
<th>Sample No.</th>
<th>Mass (g)</th>
<th>Dense bulk density (kg/m³)</th>
<th>Mean value (kg/m³)</th>
<th>Standard deviation (kg/m³)</th>
<th>CoV (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CornA</td>
<td>1</td>
<td>882</td>
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<td></td>
</tr>
<tr>
<td></td>
<td>2</td>
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<td>877</td>
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<td></td>
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<td>870</td>
<td>870</td>
<td>876</td>
<td>6</td>
<td>0.7</td>
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<td>841</td>
<td>841</td>
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</tr>
<tr>
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<td>845</td>
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<td>812</td>
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<td>0.3</td>
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<td>860</td>
<td>860</td>
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<tr>
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</table>
Table A.13 Specific weight for wheat grains

<table>
<thead>
<tr>
<th>Sample No.</th>
<th>50 grain mass (g)</th>
<th>50 grain volume (ml)</th>
<th>Specific weight (N/m³)</th>
<th>Mean value (N/m³)</th>
<th>Standard deviation (N/m³)</th>
<th>CoV (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.3291</td>
<td>1.8</td>
<td>12694</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>2.3581</td>
<td>1.8</td>
<td>12852</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>2.2887</td>
<td>1.8</td>
<td>12473</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>2.3910</td>
<td>1.9</td>
<td>12345</td>
<td>12591</td>
<td>226</td>
<td>1.8</td>
</tr>
</tbody>
</table>

Table A.14 Loose bulk densities for wheat grains

<table>
<thead>
<tr>
<th>Sample No.</th>
<th>Mass (g)</th>
<th>Loose bulk density (kg/m³)</th>
<th>Mean value (kg/m³)</th>
<th>Standard deviation (kg/m³)</th>
<th>CoV (%)</th>
<th>Void ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>717</td>
<td>717</td>
<td>717</td>
<td>4</td>
<td>0.6</td>
<td>0.441</td>
</tr>
<tr>
<td>2</td>
<td>719</td>
<td>719</td>
<td>719</td>
<td>4</td>
<td>0.6</td>
<td>0.441</td>
</tr>
<tr>
<td>3</td>
<td>712</td>
<td>712</td>
<td>712</td>
<td>4</td>
<td>0.6</td>
<td>0.441</td>
</tr>
<tr>
<td>4</td>
<td>722</td>
<td>722</td>
<td>717</td>
<td>4</td>
<td>0.6</td>
<td>0.441</td>
</tr>
</tbody>
</table>
### Table A.15 Dense bulk densities for wheat grains

<table>
<thead>
<tr>
<th>Sample No.</th>
<th>Mass (g)</th>
<th>Dense bulk density (kg/m³)</th>
<th>Mean value (kg/m³)</th>
<th>Standard deviation (kg/m³)</th>
<th>CoV (%)</th>
<th>Void ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>792</td>
<td>792</td>
<td>792</td>
<td>3</td>
<td>0.4</td>
<td>0.383</td>
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<tr>
<td>2</td>
<td>790</td>
<td>790</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
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<td></td>
<td></td>
<td></td>
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<tr>
<td>4</td>
<td>796</td>
<td>796</td>
<td>792</td>
<td>3</td>
<td>0.4</td>
<td>0.383</td>
</tr>
</tbody>
</table>

### Table A.16 Specific weight for the Garst corns

<table>
<thead>
<tr>
<th>Sample No.</th>
<th>10 grain mass (g)</th>
<th>10 grain volume (ml)</th>
<th>Specific weight (N/m³)</th>
<th>Mean value (N/m³)</th>
<th>Standard deviation (N/m³)</th>
<th>CoV (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4.2656</td>
<td>3.4</td>
<td>12491</td>
<td>12577</td>
<td>135</td>
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</tr>
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<td>2</td>
<td>4.3072</td>
<td>3.4</td>
<td>12538</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>4.2101</td>
<td>3.3</td>
<td>12515</td>
<td></td>
<td></td>
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<tr>
<td>4</td>
<td>4.0505</td>
<td>3.1</td>
<td>12818</td>
<td></td>
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<td>5</td>
<td>4.0855</td>
<td>3.2</td>
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</table>
A.2 Mechanical properties

The measurements of the mechanical properties for different type of grains are listed below (summarised in Section 5.3).
Table A.17 Young’s moduli for six types of corn grains based on the ASAE indenter method

<table>
<thead>
<tr>
<th>Corn type</th>
<th>Sample No.</th>
<th>Normal contact displacement (mm)</th>
<th>Young’s modulus (MPa)</th>
<th>Average Young’s modulus (MPa)</th>
<th>Shape description</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>CornA</td>
<td>1</td>
<td>0.069</td>
<td>775</td>
<td></td>
<td>A little flat</td>
<td>Spherical indenter can be trialed</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>0.057</td>
<td>1026</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>0.062</td>
<td>905</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CornB</td>
<td>1</td>
<td>Non</td>
<td>Non</td>
<td>900</td>
<td>Not flat</td>
<td>Spherical indenter can not be trialed</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>Non</td>
<td>Non</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>Non</td>
<td>Non</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CornC</td>
<td>1</td>
<td>Non</td>
<td>Non</td>
<td></td>
<td>Not flat</td>
<td>Spherical indenter can not be trialed</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>Non</td>
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<td></td>
<td></td>
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</tr>
<tr>
<td></td>
<td>3</td>
<td>Non</td>
<td>Non</td>
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<td></td>
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</tr>
<tr>
<td>CornD</td>
<td>1</td>
<td>Non</td>
<td>Non</td>
<td></td>
<td>Not flat</td>
<td>Spherical indenter can not be trialed</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>Non</td>
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<td></td>
<td></td>
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</tr>
<tr>
<td>CornE</td>
<td>1</td>
<td>Non</td>
<td>Non</td>
<td></td>
<td>Not flat</td>
<td>Spherical indenter can not be trialed</td>
</tr>
<tr>
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<td>Non</td>
<td>Non</td>
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</tr>
<tr>
<td>CornF</td>
<td>1</td>
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<td>1242</td>
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<td>A little flat</td>
<td>Spherical indenter can be trialed</td>
</tr>
<tr>
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<td>2</td>
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<td>0.063</td>
<td>873</td>
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</table>
Table A.18 Young’s moduli for six types of corn grains based on the proposed rigid platen compression method

<table>
<thead>
<tr>
<th>Corn type</th>
<th>Sample No.</th>
<th>Normal contact displacement (mm)</th>
<th>Radii of curvature (mm)</th>
<th>Young’s modulus (MPa)</th>
<th>Average Young’s modulus (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Longer radius</td>
<td>Shorter radius</td>
<td></td>
</tr>
<tr>
<td>CornA</td>
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<td>0.038</td>
<td>4.6</td>
<td>1.7</td>
<td>1086</td>
</tr>
<tr>
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<td>2</td>
<td>0.023</td>
<td>10.5</td>
<td>1.9</td>
<td>1772</td>
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<td></td>
<td>3</td>
<td>0.022</td>
<td>34.6</td>
<td>5.2</td>
<td>1109</td>
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<tr>
<td>CornB</td>
<td>1</td>
<td>0.027</td>
<td>3.0</td>
<td>1.2</td>
<td>2281</td>
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<td>0.027</td>
<td>2.5</td>
<td>0.9</td>
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<td>0.028</td>
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<td>1.8</td>
<td>2222</td>
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<tr>
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<td>2.9</td>
<td>1133</td>
</tr>
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<td>2.3</td>
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<td>2113</td>
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<td>1.6</td>
<td>2713</td>
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<td>9.4</td>
<td>2.6</td>
<td>1497</td>
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<td>1.4</td>
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<td>943</td>
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<td>0.024</td>
<td>9.7</td>
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</table>
### Table A.19 Young’s moduli for glass beads based on the proposed rigid platen compression method

<table>
<thead>
<tr>
<th>Sample No.</th>
<th>Displacement (mm)</th>
<th>Force (N)</th>
<th>Radius (mm)</th>
<th>Young’s modulus (GPa)</th>
<th>Mean value (GPa)</th>
<th>CoV (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.140</td>
<td>1998</td>
<td>5.00</td>
<td>40.7</td>
<td></td>
<td></td>
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<td>2</td>
<td>0.144</td>
<td>2004</td>
<td>5.00</td>
<td>39.1</td>
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<tr>
<td>3</td>
<td>0.137</td>
<td>2012</td>
<td>5.00</td>
<td>42.7</td>
<td>40.8</td>
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</table>

### Table A.20 Young’s moduli for wheat grains based on the ASAE standard (parallel plate contact)

<table>
<thead>
<tr>
<th>Sample NO.</th>
<th>Displ. (mm)</th>
<th>Force (N)</th>
<th>Length L (mm)</th>
<th>Height H (mm)</th>
<th>Radii of Curvature (mm)</th>
<th>Young’s modulus (MPa)</th>
<th>Mean value (MPa)</th>
<th>CoV (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.068</td>
<td>11.254</td>
<td>6.09</td>
<td>3.33</td>
<td>1.67</td>
<td>3.06</td>
<td>0.83</td>
<td>6.11</td>
</tr>
<tr>
<td>2</td>
<td>0.069</td>
<td>10.172</td>
<td>7.12</td>
<td>3.16</td>
<td>1.58</td>
<td>3.59</td>
<td>0.79</td>
<td>7.17</td>
</tr>
<tr>
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<td>0.067</td>
<td>9.467</td>
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<td>1.48</td>
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<td>1.70</td>
<td>3.50</td>
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</tr>
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<td>0.066</td>
<td>10.349</td>
<td>6.94</td>
<td>3.23</td>
<td>1.62</td>
<td>3.48</td>
<td>0.81</td>
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</tr>
<tr>
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<td>0.067</td>
<td>12.177</td>
<td>6.65</td>
<td>3.24</td>
<td>1.62</td>
<td>3.33</td>
<td>0.81</td>
<td>6.65</td>
</tr>
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<td>7</td>
<td>0.077</td>
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<td>6.93</td>
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<td>3.47</td>
<td>0.81</td>
<td>6.95</td>
</tr>
<tr>
<td>8</td>
<td>0.078</td>
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<td>6.72</td>
<td>2.93</td>
<td>1.47</td>
<td>3.39</td>
<td>0.73</td>
<td>6.78</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>R1 = H/2</th>
<th>R1’ = (H<em>H + 0.25</em>L<em>L)/(2</em>H)</th>
<th>R2 = 0.5*R1</th>
<th>R2’ = 2*R1’</th>
</tr>
</thead>
</table>

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Table A.21 Particle-surface friction coefficients for the six corn types on an aluminium plate (Part I)

<table>
<thead>
<tr>
<th>Corn type</th>
<th>Sample No.</th>
<th>Test No.</th>
<th>Friction Coeff.</th>
<th>Mean value for each sample</th>
<th>CoV (%) for each sample</th>
<th>Mean value for each type</th>
<th>CoV (%) for each type</th>
</tr>
</thead>
<tbody>
<tr>
<td>CornA</td>
<td>1</td>
<td>1</td>
<td>0.237</td>
<td></td>
<td></td>
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</tr>
<tr>
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<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>2</td>
<td>0.241</td>
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<td></td>
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<tr>
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Table A.23 Particle-surface friction coefficients for Garst corn grains on an acrylic plate

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Table A.24 Particle-surface friction coefficients for the wheat grains on an acrylic plate

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Table A.25 Particle-surface friction coefficients for the glass beads on an acrylic plate

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Table A.26 Particle-surface normal restitution coefficients for the glass beads on an acrylic plate

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Table A.28 Particle-surface resultant restitution coefficients for Garst corn grains on an acrylic plate

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**Table A.29** Particle-surface restitution coefficients for the medicine tablets on an acrylic plate

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<th>V_y (m/sec)</th>
<th>V_z (m/sec)</th>
<th>W_x (rad/sec)</th>
<th>W_y (rad/sec)</th>
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<th>Resultant resti. coeff.</th>
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Appendix B

Instron machine

B.1 System overview

The Instron machine (Model 4500 Testing System) at the University of Edinburgh, as shown in Figure B.1, is designed to test the physical properties of a wide range of materials, such as metals, concrete, ceramics, textiles. This system consists of three main components, i.e. a load frame, a tower console and a front panel. The system applies loads to a specimen of the material under test using a moving crosshead mounted in a rigid load frame. These loads are applied as tensile, compressive, or reverse stress loads. Testing of properties such as tensile strength, compressive strength, shear strength, torsion strength, crack growth resistance, bend characteristics etc. can be conducted with the addition of suitable purpose built loading frames.

B.2 Detailed description

During a loading test, the measurements that this system basically provides are the load upon the specimen and the position of the crosshead in response to the applied load (i.e. the force-displacement data), which may be sufficient for many tests. Three load cells with a maximum capacity of 100KN, 1KN, and 10N respectively are available. The accuracy of the load weighing system is ± 0.002% of the load cell capacity or ± 0.5% of reading whichever gives greater error. Hence, the accuracy for
different load cells is as given in Table B.1. For the single particle compression test, the appropriate load cell can be selected according to the strength of the particle. The resolution of extension measurement (relative movement of crosshead) is ±0.001 mm or ± 0.1% of reading whichever is greater.

![Figure B.1 Instron machine](image)

The straining rate can be set at any value up to 1000 mm/min, but the actual maximum loading rate that can be applied to a specimen will depend on various factors, such as the stiffness of the specimen and safety considerations. A maximum sampling rate of 50 Hz is available. In addition, this system is calibrated once a year and can be as a device for calibrating the load cells in the confined compression tester.

Table B.1 Accuracy for different load cells in the Instron machine

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<th>10N</th>
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<td>+/- 0.0002N</td>
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Appendix C

3D laser scanner

C.1 System overview

A 3D laser scanner can be used to scan a wide variety of objects. Some applications include scanning of museum artefacts for display in virtual environments, 3D objects for multimedia applications, human or animal body parts, clothing and fabrics, scanning of skulls and geological specimens. The 3D laser scanner at the University of Edinburgh (ModelMaker system), as shown in Figure C.1, consists mainly of a laser sensor, a localizer (Faro Silver arm), a ModelMaker Interface Box (MMIB), a SURFA PC board, footswitches, and sensor and video cables. It is a class 3A laser apparatus and a schematic diagram is illustrated in Figure C.2.

The object to be scanned is placed on a flat surface (or turntable) and the sensor at the end of the arm is manually moved over the whole of the object. The scanning time is dependent on the type and size of the object. The system is capable of capturing the three-dimensional surface geometry of a wide variety of items rapidly and to a high degree of resolution.

C.2 Detailed description

The sensor, mounted on a manually operated position sensing localizer, has a laser diode and stripe generator. Sensor volumetric stability is the accuracy of the sensor
for measuring features at all sensor orientations in space. The volumetric stability of this sensor is 0.1 mm. In addition, this system has four different laser power settings that make it possible to scan darker surfaces. Faro Silver arm with the accuracy of 0.04 mm is chosen as a localizer and sensor volumetric stability is 0.1 mm. Accordingly, the resolution of this system is 0.1 mm. The footswitches are used for menu control during alignment and scanning.

The image processing board (SURFA) —a full size plug-in board, in conjunction with CCD video sensor and light stripe generator, allows rapid 3D surface measurement. High speed processing of video data using a digital signal processor (DSP) on the SURFA board enables real time capture of surface depth to 16-bit resolution at over 14,000 points per second.

The sensors provided with the 3D scanner systems work on the principle of laser stripe triangulation. A laser diode and stripe generator is used to project a laser line onto the object. The line is viewed at an angle by cameras so that height variations in the object can be seen as changes in the shape of the line. The resulting captured image of the stripe is a profile that contains the shape of the object.
Figure C.1 3D laser scanner

Figure C.2 A schematic of 3D laser scanner system
Appendix D

EDEM and PFC3D input files

The intention is not to list all the EDEM and PFC3D input files used in this study but to show some typical input files. The versions used in this study were EDEM pre-release version 2.2.20 and PFC3D version 3.0.

D.1 EDEM input files

D.1.1 Silo filling of glass beads

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<particle pos_x="0.206000" pos_y="0.100000" pos_z="1.196000" vel_x="0.000000" vel_y="0.000000" vel_z="-2.562000" angvel_x="0.000000" angvel_y="0.000000" angvel_z="0.000000" orient_xx="0" orient_xy="0" orient_xz="0" orient_yx="1" orient_yy="0" orient_yz="0" orient_zx="0" orient_zy="0" orient_zz="1" scaling_factor="1" id="3571" type="balla"/>

<particle pos_x="0.148000" pos_y="0.164000" pos_z="1.206000" vel_x="0.000000" vel_y="0.000000" vel_z="-2.562000" angvel_x="0.000000" angvel_y="0.000000" angvel_z="0.000000" orient_xx="0" orient_xy="0" orient_xz="0" orient_yx="1" orient_yy="0" orient_yz="0" orient_zx="0" orient_zy="0" orient_zz="1" scaling_factor="1" id="3572" type="balla"/>

<particle pos_x="0.148000" pos_y="0.132000" pos_z="1.206000" vel_x="0.000000" vel_y="0.000000" vel_z="-2.562000" angvel_x="0.000000" angvel_y="0.000000" angvel_z="0.000000" orient_xx="0" orient_xy="0" orient_xz="0" orient_yx="1" orient_yy="0" orient_yz="0" orient_zx="0" orient_zy="0" orient_zz="1" scaling_factor="1" id="3573" type="balla"/>

<particle pos_x="0.148000" pos_y="0.100000" pos_z="1.206000" vel_x="0.000000" vel_y="0.000000" vel_z="-2.562000" angvel_x="0.000000" angvel_y="0.000000" angvel_z="0.000000" orient_xx="0" orient_xy="0" orient_xz="0" orient_yx="1" orient_yy="0" orient_yz="0" orient_zx="0" orient_zy="0" orient_zz="1" scaling_factor="1" id="3574" type="balla"/>

<particle pos_x="0.148000" pos_y="0.116000" pos_z="1.206000" vel_x="0.000000" vel_y="0.000000" vel_z="-2.562000" angvel_x="0.000000" angvel_y="0.000000" angvel_z="0.000000" orient_xx="0" orient_xy="0" orient_xz="0" orient_yx="1" orient_yy="0" orient_yz="0" orient_zx="0" orient_zy="0" orient_zz="1" scaling_factor="1" id="3575" type="balla"/>

<particle pos_x="0.148000" pos_y="0.196000" pos_z="1.206000" vel_x="0.000000" vel_y="0.000000" vel_z="-2.562000" angvel_x="0.000000" angvel_y="0.000000" angvel_z="0.000000" orient_xx="0" orient_xy="0" orient_xz="0" orient_yx="1" orient_yy="0" orient_yz="0" orient_zx="0" orient_zy="0" orient_zz="1" scaling_factor="1" id="3576" type="balla"/>
<simulation>
  <particles>
    <particle pos_x=".132000" pos_y=".164000" pos_z="1.206000" vel_x=".000000" vel_y=".000000" vel_z=".000000">
      <material shear_modulus="1.074e+9" name="elastic_sphere" poissons_ratio="0.22" density="2530" />
    </particle>
    <particle pos_x=".164000" pos_y=".132000" pos_z="1.206000" vel_x=".000000" vel_y=".000000" vel_z=".000000">
      <material shear_modulus="1.673e+10" name="elastic_sphere" poissons_ratio="0.35" density="1190" />
    </particle>
    <material shear_modulus="1.074e+9" name="container" poissons_ratio="0.35" density="1190" />
    <interaction material1="elastic_sphere" material2="container" coeff_friction="0.244" coeff_restitution="0.793" />
    <interaction material1="elastic_sphere" material2="elastic_sphere" coeff_friction="0.244" coeff_restitution="0.793" />
  </particles>
  <materials>
    <material shear_modulus="1.074e+9" name="container" poissons_ratio="0.35" density="1190" />
  </materials>
</simulation>
D.1.2 Silo discharge of glass beads

<simulation dimensions="3" phases='1' version='2.2.20' name="Glassbeads_discharge_orifice_0.6D" date="12/12/04">
  <globals>
    <gravity x="0" y="0" z="9.811"/>
  </globals>
  <materials>
    <material poissons_ratio="0.35" density="1190" shear_modulus="1.074e+09" name="container"/>
    <material poissons_ratio="0.22" density="2510" shear_modulus="1.673e+10" name="elastic_sphere"/>
    <material poissons_ratio="0.35" density="1190" shear_modulus="1.074e+09" name="load_cell"/>
  </materials>
  <interactions>
    <interaction coeff_friction="0.244" coeff_restitution="0.793" material1="elastic_sphere" material2="container"/>
    <interaction coeff_friction="0.244" coeff_restitution="0.793" material1="elastic_sphere" material2="container"/>
    <interaction coeff_friction="0.244" coeff_restitution="0.793" material1="elastic_sphere" material2="load_cell"/>
  </interactions>
</simulation>
D.2 PFC3D input files

D.2.1 Confined compression of corn grains

```plaintext
Corn_Filling_G_1.50d_WallFric_0.335_PartFric_0.335_1.dat
new
title 'Corn_Filling_G_1.50d_WallFric_0.335_PartFric_0.335'
; set echo on
set log on
set logfile Logfile_Filling_1
trace energy on
set pinterval 2000
set hist_rep 2000
set plot bmp
;
define model-parameter
 ; Particle property
  Shear_modulus= 5.92857e+08
  Poisson_ratio= 0.4
  Par_fric= 0.335
  Damping_ratio= 0.212
  Par_den= 1280
; Wall property
  CylinderRadius= 0.0725
  CylinderCrossArea=\pi*CylinderRadius*CylinderRadius
  Wall_fric= 0.335
end
model-parameter
;
damp default local 0.0
damp default viscous normal Damping_ratio
damp default viscous shear Damping_ratio
;
call PFC_Wall_Data.dat
wall property friction Wall_fric
;
call Corn_ParticleGeneration.dat
ParticleGeneration
SetupVelocity
CountClumps
pause
;
define currenttime
  while stepping
    currenttime=time
  end
;
set gravity 0.0 0.0 -9.81
set safety_fac 0.20
;
plot create FillingModel
plot set center auto
plot set distance auto
plot add wall wireframe on
plot add clump yellow
plot show
;
plot create VelocityDiagram
plot set center auto
plot set distance auto
plot add wall wireframe on
plot add clump yellow
plot add velocity
plot show
;
history id 1 currenttime
history id 2 diagnostic mcf
history id 3 diagnostic muf
```
history id 4 energy kinetic
plot create MCF_MUF_Diagram
plot add history 2, 3
plot set title text 'Monitoring MCF and MUF'
plot show

plot create KineticEnergyDiagram
plot add history 4
plot set title text 'Monitoring Kinetic Energy'
plot show

cycle 500000
history write 1 2 3 4 file Results_MCF_MUF_KineticJ HIS
save Output_files\Corn_Filling_G_1.50d_WallFric_0.335_PartFric_0.335_1.sav
return

PFC_WaILData.dat

wall id 1 face .142214E-01 .282881E-02 .000000E+00 .133963E-01 .554891E-02 .000000E+00 .000000E+00 .000000E+00 .000000E+00
wall id 2 face .133963E-01 .554891E-02 .000000E+00 .120563E-01 .805577E-02 .000000E+00 .000000E+00 .000000E+00 .000000E+00
wall id 3 face .120563E-01 .805577E-02 .000000E+00 .102530E-01 .102530E-01 .000000E+00 .000000E+00 .000000E+00 .000000E+00
wall id 4 face .102530E-01 .102530E-01 .000000E+00 .805577E-02 .120563E-01 .000000E+00 .000000E+00 .000000E+00 .000000E+00
wall id 5 face .805577E-02 .120563E-01 .000000E+00 .554891E-02 .133963E-01 .000000E+00 .000000E+00 .000000E+00 .000000E+00
wall id 6 face .554891E-02 .133963E-01 .000000E+00 .282881E-02 .142214E-01 .000000E+00 .000000E+00 .000000E+00 .000000E+00
wall id 7 face .282881E-02 .142214E-01 .000000E+00 -.633815E-09 .145000E-01 .000000E+00 .000000E+00 .000000E+00 .000000E+00
wall id 8 face -.633815E-09 .145000E-01 .000000E+00 -.282881E-02 .142214E-01 .000000E+00 .000000E+00 .000000E+00 .000000E+00
wall id 9 face -.282881E-02 .142214E-01 .000000E+00 -.554891E-02 .133963E-01 .000000E+00 .000000E+00 .000000E+00 .000000E+00
wall id 10 face -.554891E-02 .133963E-01 .000000E+00 -.805577E-02 .120563E-01 .000000E+00 .000000E+00 .000000E+00 .000000E+00
wall id 11 face -.805577E-02 .120563E-01 .000000E+00 -.102530E-01 .102530E-01 .000000E+00 .000000E+00 .000000E+00 .000000E+00
wall id 12 face -.102530E-01 .102530E-01 .000000E+00 -.120563E-01 .805577E-02 .000000E+00 .000000E+00 .000000E+00 .000000E+00
wall id 13 face -.120563E-01 .805577E-02 .000000E+00 -.133963E-01 .554891E-02 .000000E+00 .000000E+00 .000000E+00 .000000E+00
wall id 14 face -.133963E-01 .554891E-02 .000000E+00 -.142214E-01 .282881E-02 .000000E+00 .000000E+00 .000000E+00 .000000E+00
wall id 15 face -.142214E-01 .282881E-02 .000000E+00 -.145000E-01 -.145000E-01 .000000E+00 .000000E+00 .000000E+00 .000000E+00
wall id 16 face -.145000E-01 -.145000E-01 .000000E+00 -.142214E-01 -.282881E-02 .000000E+00 .000000E+00 .000000E+00 .000000E+00
wall id 17 face -.142214E-01 -.282881E-02 .000000E+00 -.133963E-01 -.554891E-02 .000000E+00 .000000E+00 .000000E+00 .000000E+00
wall id 18 face -.133963E-01 -.554891E-02 .000000E+00 -.120563E-01 -.805577E-02 .000000E+00 .000000E+00 .000000E+00 .000000E+00
wall id 19 face -.120563E-01 -.805577E-02 .000000E+00 -.102530E-01 -.102530E-01 .000000E+00 .000000E+00 .000000E+00 .000000E+00
wall id 20 face -.102530E-01 -.102530E-01 .000000E+00 -.805577E-02 -.120563E-01 .000000E+00 .000000E+00 .000000E+00 .000000E+00
wall id 21 face -.805577E-02 -.120563E-01 .000000E+00 -.554891E-02 -.133963E-01 .000000E+00 .000000E+00 .000000E+00 .000000E+00
wall id 22 face -.554891E-02 -.133963E-01 .000000E+00 -.282881E-02 -.142214E-01 .000000E+00 .000000E+00 .000000E+00 .000000E+00
wall id 23 face -.282881E-02 -.142214E-01 .000000E+00 .190145E-08 -.145000E-01 .000000E+00 .000000E+00 .000000E+00 .000000E+00
wall id 24 face .190145E-08 -.145000E-01 .000000E+00 .282881E-02 -.142214E-01 .000000E+00 .000000E+00 .000000E+00 .000000E+00
wall id 25 face .282881E-02 -.142214E-01 .000000E+00 .554891E-02 -.133963E-01 .000000E+00 .000000E+00 .000000E+00 .000000E+00
wall id 26 face .554891E-02 -.133963E-01 .000000E+00 .805577E-02 -.120563E-01 .000000E+00 .000000E+00 .000000E+00 .000000E+00

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Corn_ParticleGeneration.dat

define ParticleGeneration

;Initial parameters
X0= 0.0
Y0=0.0
Z0= 0.007
OverallRadius= 0.006
ParticleSpacing= 0.015165
ParticleOffset= 0.001
MaxNumber= 60
LayerNumber= 200
SegmentNumber= 32
InitialVel_z= -2.562

MeshRadius=CylinderRadius*cos(pi/SegmentNumber)

GivenNumber=4672

section
loop k (1, LayerNumber)
  Cenz=Z0+ParticleSpacing*(k-1)
  loop i (1, MaxNumber)
    Cenx=X0+CylinderRadius+i*ParticleSpacing+ParticleOffset*(-1)*(k-1)
    loop j (1, MaxNumber)
      Ceny=Y0+CylinderRadius+j*ParticleSpacing+ParticleOffset*(-1)*(k-1)
      RelativeDistance=sqrt((Cenx-X0)**2+(Ceny-Y0)**2)+OverallRadius
      if RelativeDistance < MeshRadius then
        _mid=_mid+1
        make(grain)
      end_if
    end_loop
  end_if
end_loop
end_section

end

define CountClumps
_clk = 0
loop while _clk # null
  _cnt = _cnt + 1
  _clk = cl_next(_clk)
end_loop
jj = out("The number of particles = " + ' + string(_cnt))
end

define SetupVelocity
_clp = clump_head
loop
  _clp = cl_next(_clp)
end

282
loop while clp # null
    cl_zvel(clp)= Initial Vel_z
    jj = out('The ID number = ' + string(cl_id(clp))+ ' 
' + string(cl_zvel(clp)))
    clp = cl_next(clp)
end_loop

define make_grain
    _bid = max_bid
    _bid0 = max_bid + 1
    _bid = _bid + 1
    _x = Cenx+0.00121
    _y = Ceny+0.0
    _z = Cenz-0.001419
    command
        ball id=_bid hertz x=_x y=_y z=_z rad= 0.003345
    end_command
    _bid = _bid + 1
    _x = Cenx-0.00121
    _y = Ceny+0.0
    _z = Cenz-0.001419
    command
        ball id=_bid hertz x=_x y=_y z=_z rad= 0.003345
    end_command
    _bid = _bid + 1
    _x = Cenx+0.0008
    _y = Ceny+0.0
    _z = Cenz+0.002346
    command
        ball id=_bid hertz x=_x y=_y z=_z rad= 0.003
    end_command
    _bid = _bid + 1
    _x = Cenx-0.0008
    _y = Ceny+0.0
    _z = Cenz+0.002346
    command
        ball id=_bid hertz x=_x y=_y z=_z rad= 0.003
    end_command
    _bid1 = _bid
    command
        clump id=_mid range id=_bid0,_bid1
        property shear Shear_modulus poiss Poisson_ratio friction Par_fric density Par_den range id=_bid0,_bid1
end_command
end

Corn_Ko_G_1.50d_WallFric_0.335_PartFric_0.335_1.dat
new
restore Output_filesCom_FiIling_G_l .50d_WalIFric_0.335_PartFric_0.335_l .sav
set echo on
set log on
set logfile Logfile_Compression_1

damp default local 0.0
damp default viscous normal Damping_ratio
damp default viscous shear Damping_ratio
;print information
;pause

define model_parameter_2
;System information
    SystemWeight= -GivenNumber*6.660980e-3
;lid information
LidID = 2000
HighestPoint = 0.0
Lid_Xmax = CylinderRadius + 0.010
Lid_Xmin = -Lid_Xmax
Lid_Ymax = CylinderRadius + 0.010
Lid_Ymin = -Lid_Ymax
DisplacementRate = -8.333e-4

; resultant force calculation
bottom_begin = 1
bottom_end = 224
cylinder_begin = 225
cylinder_end = 864

; pressure calculation
SectionHeight = 0.3 / 15.0
SectionArea = 2.0 * CylinderRadius * sin(pi/SegmentNumber) * SegmentNumber * SectionHeight
UpdateCounter = 0
Update_Counter = 0
UpdateCycles = 20000

end
model_parameter_2,
CountClumps
pause
plot create Ko_ForceChain
plot set center auto
plot set distance auto
plot add wall wireframe on
plot add clump yellow
plot add cforce red
plot show

call Measure_Sphere.dat

define FindHighestPoint
clp = clump_head
loop while clp # null
   HeightParticle = cl_z(clp) + 5.0e-03
   if HeightParticle > HighestPoint then
      HighestPoint = HeightParticle
   end_if
   clp = cl_next(clp)
end_loop
ii = out(string(HighestPoint))
end
FindHighestPoint

WALL id LidID face (Lid_Xmax, Lid_Ymax, HighestPoint) (Lid_Xmax, Lid_Ymin, HighestPoint) &
(Lid_Xmin, Lid_Ymin, HighestPoint) (Lid_Xmin, Lid_Ymax, HighestPoint)
WALL property friction Wall_fric zvelocity DisplacementRate id LidID
print walls velocity

call Fz_Calculation.dat
FzCalculation

call Pressure_Calculation.dat
PressureCalculation

call Stress_Porosity_Calculation.dat
StressPorosityCalculation

history id 5 Fz_Bottom
history id 6 Fz_Cylinder
history id 7 Fz_Top

plot create TopForceDiagram
plot add history 7
plot set title text 'Monitoring the top force'
plot show

cycle 3000000
history write 1 5 6 7 file Results_1_resultant_z_force.HIS
Measure_Sphere.dat
measure id 1 x 0.0000 y 0.0000 z 0.02 radius 0.02
measure id 2 x 0.0000 y 0.0000 z 0.04 radius 0.02
measure id 3 x 0.0000 y 0.0000 z 0.06 radius 0.02
measure id 4 x 0.0000 y 0.0000 z 0.08 radius 0.02
measure id 5 x 0.0000 y 0.0000 z 0.10 radius 0.02
measure id 6 x 0.0000 y 0.0000 z 0.12 radius 0.02
measure id 7 x 0.0000 y 0.0000 z 0.14 radius 0.02
measure id 8 x 0.0525 y 0.0000 z 0.02 radius 0.02
measure id 9 x 0.0525 y 0.0000 z 0.04 radius 0.02
measure id 10 x 0.0525 y 0.0000 z 0.06 radius 0.02
measure id 11 x 0.0525 y 0.0000 z 0.08 radius 0.02
measure id 12 x 0.0525 y 0.0000 z 0.10 radius 0.02
measure id 13 x 0.0525 y 0.0000 z 0.12 radius 0.02
measure id 14 x 0.0525 y 0.0000 z 0.14 radius 0.02
measure id 15 x -0.0525 y 0.0000 z 0.02 radius 0.02
measure id 16 x -0.0525 y 0.0000 z 0.04 radius 0.02
measure id 17 x -0.0525 y 0.0000 z 0.06 radius 0.02
measure id 18 x -0.0525 y 0.0000 z 0.08 radius 0.02
measure id 19 x -0.0525 y 0.0000 z 0.10 radius 0.02
measure id 20 x -0.0525 y 0.0000 z 0.12 radius 0.02
measure id 21 x -0.0525 y 0.0000 z 0.14 radius 0.02
measure id 22 x -0.0350 y 0.0000 z 0.02 radius 0.02
measure id 23 x -0.0350 y 0.0000 z 0.04 radius 0.02
measure id 24 x -0.0350 y 0.0000 z 0.06 radius 0.02
measure id 25 x -0.0350 y 0.0000 z 0.08 radius 0.02
measure id 26 x -0.0350 y 0.0000 z 0.10 radius 0.02
measure id 27 x -0.0350 y 0.0000 z 0.12 radius 0.02
measure id 28 x -0.0350 y 0.0000 z 0.14 radius 0.02
measure id 29 x -0.0175 y 0.0000 z 0.02 radius 0.02
measure id 30 x -0.0175 y 0.0000 z 0.04 radius 0.02
measure id 31 x -0.0175 y 0.0000 z 0.06 radius 0.02
measure id 32 x -0.0175 y 0.0000 z 0.08 radius 0.02
measure id 33 x -0.0175 y 0.0000 z 0.10 radius 0.02
measure id 34 x -0.0175 y 0.0000 z 0.12 radius 0.02
measure id 35 x -0.0175 y 0.0000 z 0.14 radius 0.02
measure id 36 x 0.0175 y 0.0000 z 0.02 radius 0.02
measure id 37 x 0.0175 y 0.0000 z 0.04 radius 0.02
measure id 38 x 0.0175 y 0.0000 z 0.06 radius 0.02
measure id 39 x 0.0175 y 0.0000 z 0.08 radius 0.02
measure id 40 x 0.0175 y 0.0000 z 0.10 radius 0.02
measure id 41 x 0.0175 y 0.0000 z 0.12 radius 0.02
measure id 42 x 0.0175 y 0.0000 z 0.14 radius 0.02
measure id 43 x 0.0350 y 0.0000 z 0.02 radius 0.02
measure id 44 x 0.0350 y 0.0000 z 0.04 radius 0.02
measure id 45 x 0.0350 y 0.0000 z 0.06 radius 0.02
measure id 46 x 0.0350 y 0.0000 z 0.08 radius 0.02
measure id 47 x 0.0350 y 0.0000 z 0.10 radius 0.02
measure id 48 x 0.0350 y 0.0000 z 0.12 radius 0.02
measure id 49 x 0.0350 y 0.0000 z 0.14 radius 0.02

Fz_Calculation.dat
define FzCalculation
whilestepping
Fz_Sum=0.0
wp=wall_head
loop while wp # null
  if w_id(wp) >= bottom_begin then
    if w_id(wp) <= bottom_end then
      Fz_Sum=Fz_Sum+w_zfob(wp)
    end if
  end if
  wp=w_next(wp)
end_loop
Fz_Bottom= Fz_Sum
Fz_Sum=0.0
wp=wall_head
loop while wp # null
  if w_id(wp) >= cylinder_begin then
    if w_id(wp) <= cylinder_end then
      Fz_Sum = Fz_Sum + w_zfob(wp)
    end if
  end if
  wp = w_next(wp)
end loop
Fz_Cylinder = Fz_Sum
Fz_Top = w_zfob(find_wall(LidID))
end

Pressure_Calculation.dat
define PressureCalculation
  status = open("WallPressure_Stress_Porosity.fio", 1, 1)
  array MessageLine(1)
  if UpdateCounter = 0 then
    UpdateCounter = UpdateCycles
  end if
  command
    set fishcall 0 CheckExecution
  end_command
end

define CheckExecution
  if UpdateCounter = 0 then
    UpdateCounter = UpdateCycles
  end if
  if UpdateCounter = UpdateCycles then
    UpdateCounter = 0
    ComputePressure
  end if
  UpdateCounter = UpdateCounter + 1
end

define ComputePressure
  array CircumForce(10, 2)
  array Pressure(10, 2)
  array SumHS(2)
  loop iii (1, 10)
    loop jjj (1, 2)
      CircumForce(iii, jjj) = 0.0
      Pressure(iii, jjj) = 0.0
    end_loop
  end_loop
  loop iii (1, 2)
    SumHS(iii) = 0.0
  end_loop
  cp = contact_head
  loop while cp # null
    EntityB = c_ball2(cp)
    if pointer_type(EntityB) = 101 then
      if w_id(EntityB) >= 225 then
        if w_id(EntityB) <= 864 then
          caseof (w_id(EntityB) - 224 - 1)
            CircumForce(1, 1) = CircumForce(1, 1) + c_nforce(cp)
            CircumForce(1, 2) = CircumForce(1, 2) + c_zsforce(cp)
            case 1
              CircumForce(2, 1) = CircumForce(2, 1) + c_nforce(cp)
              CircumForce(2, 2) = CircumForce(2, 2) + c_zsforce(cp)
            case 2
              CircumForce(3, 1) = CircumForce(3, 1) + c_nforce(cp)
              CircumForce(3, 2) = CircumForce(3, 2) + c_zsforce(cp)
            case 3
  ...
CircumForce(4, 1) = CircumForce(4, 1) + c_nforce(cp)
CircumForce(4, 2) = CircumForce(4, 2) + c_zsforce(cp)

case 4
CircumForce(5, 1) = CircumForce(5, 1) + c_nforce(cp)
CircumForce(5, 2) = CircumForce(5, 2) + c_zsforce(cp)

case 5
CircumForce(6, 1) = CircumForce(6, 1) + c_nforce(cp)
CircumForce(6, 2) = CircumForce(6, 2) + c_zsforce(cp)

case 6
CircumForce(7, 1) = CircumForce(7, 1) + c_nforce(cp)
CircumForce(7, 2) = CircumForce(7, 2) + c_zsforce(cp)

case 7
CircumForce(8, 1) = CircumForce(8, 1) + c_nforce(cp)
CircumForce(8, 2) = CircumForce(8, 2) + c_zsforce(cp)

case 8
CircumForce(9, 1) = CircumForce(9, 1) + c_nforce(cp)
CircumForce(9, 2) = CircumForce(9, 2) + c_zsforce(cp)

case 9
CircumForce(10, 1) = CircumForce(10, 1) + c_nforce(cp)
CircumForce(10, 2) = CircumForce(10, 2) + c_zsforce(cp)

case_end

end_if

cp = c_next(cp)

end_loop

loop iii (1, 10)
loop jjj (1, 2)
Pressure(iii, jjj) = CircumForce(iii, jjj)/SectionArea
end_loop
end_loop

loop iii (1, 2)
loop jjj (1, 10)
SumHS(iii) = SumHS(iii) + Pressure(jjj, iii)
end_loop
end_loop

SigmaV = 0.5*(Fz_Top - Fz_Bottom)/CylinderCrossArea
SigmaV2 = 0.5*(Fz_Top + Fz_Bottom + SystemWeight)/CylinderCrossArea
SigmaH = SumHS(1)/10.0
Tau = -SumHS(2)/10.0
KValue = SigmaH/SigmaV
KValue2 = SigmaH/SigmaV2
FricValue = Tau/SigmaH

MessageLine(1) = ('Current time= ' + string(time) + '
Top force= ' + string(Fz_Top) + '
Bottom force= ' + string(Fz_Bottom) + '
K value= ' + string(KValue) + '
Friction= ' + string(FricValue) + '
KValue2')
status = write(MessageLine, 1)

end_loop
end

Stress_Porosity_Calculation.dat
define StressPorosityCalculation
array Message_Line(1)
if Update_Counter=0 then
Update_Counter= UpdateCycles
end_if
command
set fishcall 0 Check_Execution
end_command
end

define Check_Execution
if Update_Counter=0 then
Update_Counter= UpdateCycles
end
end_if

if Update_Counter = UpdateCycles then
  Update_Counter = 0
  ComputeStressPorosity
end_if

Update_Counter = Update_Counter + 1

end

define ComputeStressPorosity
  Message_Line(1) = ('Current time= ' + \\t+ string(time) + 'W+ Top force= ' + \\t+ string(Fz_Top) )
  status = write(Message_Line,1)
  mp= circ_head
  loop while mp # null
    jj=measure(mp, 1)
    Message_Line(1) = (string(m_s11(mp))+\t'+string(m_s12(mp))+\t'+string(m_s13(mp))+\t'+string(m_s21(mp))+\t'+string(m_s22(mp))+\t'+string(m_s23(mp))+\t'+string(m_s31(mp))+\t'+string(m_s32(mp))+\t'+string(m_s33(mp))+\t'+string(m_poros(mp)))
    status = write(Message_Line,1)
    mp = m_next(mp)
  end_loop
end
D.2.2 Rod penetration of corn grains

Corn_Filling_0.01G_1.50d_WallFric_0.335_PartFric_0.335_1.dat
new
title 'Corn_Filling_0.01G_1.50d_WallFric_0.335_PartFric_0.335'
set echo on
set log on
set logfile Logfile_Filling_1
trace energy on
set pinterval 2000
set hist_rep 2000
set plot bmp

define model_parameter
;Particle property
   Shear_modulus= 5.92857e+06
   Poisson_ratio= 0.4
   Par_fric= 0.335
   Damping_ratio= 0.212
   Par_den= 1280
;Wall property
   CylinderRadius= 0.0725
   CylinderCrossArea=pi*CylinderRadius*CylinderRadius
   Wall_fric= 0.335
end
model_parameter

damp default local 0.0
damp default viscous normal Damping_ratio
damp default viscous shear Damping_ratio

call PFC_Wall_Data.dat
wall property friction Wall_fric

call Corn_ParticleGeneration.dat
ParticleGeneration
SetupVelocity
CountClumps
pause

define currenttime
   whilestepping
      currenttime=time
end

set gravity 0.0 0.0 -9.81
set safety_fac 0.20

plot create FillingModel
plot set center auto
plot set distance auto
plot add wall wireframe on
plot add clump yellow
plot show

plot create VelocityDiagram
plot set center auto
plot set distance auto
plot add wall wireframe on
plot add clump yellow
plot add velocity
plot show

history id 1 currenttime
history id 2 diagnostic mcf
history id 3 diagnostic muf
history id 4 energy kinetic

plot create MCF_MUF_Diagram
plot add history 2, 3
define ParticleGeneration
;Initial parameters
X0= 0.0
Y0= 0.0
Z0= 0.007
OverallRadius= 0.006
ParticleSpacing= 0.015165
ParticleOffset= 0.001
MaxNumber= 60
LayerNumber= 200
SegmentNumber= 32
InitialVel_z= -2.562
_Mid=0
MeshRadius=CylinderRadius*cos(pi/SegmentNumber)
GivenNumber=4672

section
loop k (1, LayerNumber)
CenZ=Z0+ParticleSpacing*(k-1)
loop i (1, MaxNumber)
CenX=X0+CylinderRadius+i*ParticleSpacing+ParticleOffset*(-1)^*(k-1)
loop j (1, MaxNumber)
Ceny=Y0-CylinderRadius+j*ParticleSpacing+ParticleOffset*(-1)^*(k-1)
RelativeDistance=sqrt((CenX-X0)^2+(Ceny-Y0)^2)+OverallRadius
if RelativeDistance < MeshRadius then
_Mid=_Mid+1
make-grain
if _Mid = GivenNumber then
exit section
end-if
end-if
end_loop
end_loop
end _loop
end-section
end

define CountClumps
_cnt = 0
clp = clump_head
loop while clp # null
_cnt = _cnt + 1
clp = cl_next(clp)
end_loop
jj = out('The number of particles = ' + _cnt + string(_cnt))
end

define SetupVelocity
clp = clump_head
loop while clp # null
cl_zvel(clp)= InitialVel_z
jj = out('The ID number = ' + _zvel + string(cl_id(clp))+ _zvel + string(cl_zvel(clp)))
clp = cl_next(clp)
end_loop
end

define make_grain

_bid = max_bid
_bid0 = max_bid + 1

_bid = _bid + 1
_x = Cenx+0.00121
_y = Ceny+0.0
_z = Cenz-0.001419
command
   ball ids _bid hertz x= _x y= _y z= _z rad= 0.003345
end_command

_bid = _bid + 1
_x = Cenx-0.00121
_y = Ceny+0.0
_z = Cenz-0.001419
command
   ball ids _bid hertz x= _x y= _y z= _z rad= 0.003345
end_command

_bid = _bid + 1
_x = Cenx+0.0008
_y = Ceny+0.0
_z = Cenz+0.002346
command
   ball ids _bid hertz x= _x y= _y z= _z rad= 0.003
end_command

_bid = _bid + 1
_x = Cenx-0.0008
_y = Ceny+0.0
_z = Cenz+0.002346
command
   ball ids _bid hertz x= _x y= _y z= _z rad= 0.003
end_command

_bidl = _bid
command
   clump id= _mid range id= _bid0, _bidl
   property shear Shear_modulus poiss Poisson_ratio friction Par_fric density Par_den range id= _bid0, _bidl
end_command

end

Corn_Pe_0.01G_1.50d_WallFric_0.335_PartFric_0.335_1.dat
new

restore Output_files\Corn_Filling_0.01G_1.50d_WallFric_0.335_PartFric_0.335_1.sav
set echo on
set log on
set logfile Logfile_Pe_1

; damp default local 0.0
damp default viscous normal Damping_ratio
damp default viscous shear Damping_ratio
; print information
; pause

define model-parameter_2
; System information
   SystemWeight= -GivenNumber*6.660980e-3
; lid information
   RodTip=0.0
   DisplacementRate= -8.333e-4
; resultant force calculation
   bottom_begin=1

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; pressure calculation
SectionHeight = 0.3 / 15.0
SectionArea = 2.0 * CylinderRadius * sin(\pi / SegmentNumber) * SegmentNumber * SectionHeight
UpdateCounter = 0
Update_Counter = 0
UpdateCycles = 50000
end
model parameter_2

plot create Pe_ForceChain
plot set center auto
plot set distance auto
plot add wall wireframe on
plot add clump yellow
plot add cforce red
plot show

call Measure_Sphere.dat

define FindHighestPoint
clp = clump_head
loop while clp # null
    ClumpDistance = sqrt(cl_x(clp) * cl_x(clp) + cl_y(clp) * cl_y(clp))
    if ClumpDistance < 0.010 then
        HeightParticle = cl_z(clp) + 0.004
        if HeightParticle > RodTip then
            RodTip = HeightParticle
        end_if
    end_if
    clp = cl_next(clp)
end_loop
ii = out('The Z coordinate of the rod tip = ' + string(RodTip))
end
FindHighestPoint
pause

call PFC_Wall_Rod_Data.dat
wall property friction Wall_fric

define RodVelocity
wp = wall_head
loop while wp # null
    if w_id(wp) >= RodBegin then
        if w_id(wp) <= RodEnd then
            w_zvel(wp) = DisplacementRate
        end_if
    end_if
    wp = w_next(wp)
end_loop
end
RodVelocity
print walls velocity
pause

call Fz_Calculation.dat
FzCalculation

call Pressure_Calculation.dat
PressureCalculation

call Stress_Porosity_Calculation.dat
StressPorosityCalculation

history id 5 Fz_Bottom
history id 6 Fz_Cylinder
history id 7 Fz_Top

plot create TopForceDiagram
plot add history 7
plot set title text 'Monitoring the top force'
plot show

cycle 7000000
history write 1 5 6 7 file Results_1_resultant_z_force.HIS
save Output_files/Corrn_Pe_0.01G_1.50d_WallFric_0.335_PartFric_0.335_1.sav
return

Measure_Sphere.dat
measure id 1 x .0000 y .0000 z .02 radius 0.02
measure id 2 x .0000 y .0000 z .04 radius 0.02
measure id 3 x .0000 y .0000 z .06 radius 0.02
measure id 4 x .0000 y .0000 z .08 radius 0.02
measure id 5 x .0000 y .0000 z .10 radius 0.02
measure id 6 x .0000 y .0000 z .12 radius 0.02
measure id 7 x .0000 y .0000 z .14 radius 0.02
measure id 8 x .0525 y .0000 z .02 radius 0.02
measure id 9 x .0525 y .0000 z .04 radius 0.02
measure id 10 x .0525 y .0000 z .06 radius 0.02
measure id 11 x .0525 y .0000 z .08 radius 0.02
measure id 12 x .0525 y .0000 z .10 radius 0.02
measure id 13 x .0525 y .0000 z .12 radius 0.02
measure id 14 x .0525 y .0000 z .14 radius 0.02
measure id 15 x -.0525 y .0000 z .02 radius 0.02
measure id 16 x -.0525 y .0000 z .04 radius 0.02
measure id 17 x -.0525 y .0000 z .06 radius 0.02
measure id 18 x -.0525 y .0000 z .08 radius 0.02
measure id 19 x -.0525 y .0000 z .10 radius 0.02
measure id 20 x -.0525 y .0000 z .12 radius 0.02
measure id 21 x -.0525 y .0000 z .14 radius 0.02
measure id 22 x -.0350 y .0000 z .02 radius 0.02
measure id 23 x -.0350 y .0000 z .04 radius 0.02
measure id 24 x -.0350 y .0000 z .06 radius 0.02
measure id 25 x -.0350 y .0000 z .08 radius 0.02
measure id 26 x -.0350 y .0000 z .10 radius 0.02
measure id 27 x -.0350 y .0000 z .12 radius 0.02
measure id 28 x -.0350 y .0000 z .14 radius 0.02
measure id 29 x -.0175 y .0000 z .02 radius 0.02
measure id 30 x -.0175 y .0000 z .04 radius 0.02
measure id 31 x -.0175 y .0000 z .06 radius 0.02
measure id 32 x -.0175 y .0000 z .08 radius 0.02
measure id 33 x -.0175 y .0000 z .10 radius 0.02
measure id 34 x -.0175 y .0000 z .12 radius 0.02
measure id 35 x -.0175 y .0000 z .14 radius 0.02
measure id 36 x .0175 y .0000 z .02 radius 0.02
measure id 37 x .0175 y .0000 z .04 radius 0.02
measure id 38 x .0175 y .0000 z .06 radius 0.02
measure id 39 x .0175 y .0000 z .08 radius 0.02
measure id 40 x .0175 y .0000 z .10 radius 0.02
measure id 41 x .0175 y .0000 z .12 radius 0.02
measure id 42 x .0175 y .0000 z .14 radius 0.02
measure id 43 x .0350 y .0000 z .02 radius 0.02
measure id 44 x .0350 y .0000 z .04 radius 0.02
measure id 45 x .0350 y .0000 z .06 radius 0.02
measure id 46 x .0350 y .0000 z .08 radius 0.02
measure id 47 x .0350 y .0000 z .10 radius 0.02
measure id 48 x .0350 y .0000 z .12 radius 0.02
measure id 49 x .0350 y .0000 z .14 radius 0.02

PFC_Wall_Rod_Data.dat
wall id 1185 face .100652E-02 .167648E+00 .000000E+00 .000000E+00 .000000E+00 .167600E+00 .770354E-03 .167648E+00
wall id 1186 face .100652E-02 .167648E+00 .000000E+00 .000000E+00 .000000E+00 .167600E+00 .770354E-03 .167648E+00
wall id 1187 face .100652E-02 .167648E+00 .000000E+00 .000000E+00 .000000E+00 .167600E+00 .770354E-03 .167648E+00
wall id 1188 face .100652E-02 .167648E+00 .000000E+00 .000000E+00 .000000E+00 .167600E+00 .770354E-03 .167648E+00
wall id 1476 face -.883883E-02 -.883884E-02 .280100E+00 -.478354E-02 -.115485E-01 .260100E+00 -.478354E-02 -.115485E-01 .280100E+00
wall id 1477 face -.478354E-02 -.115485E-01 .260100E+00 .163918E-08 -.125000E-01 .260100E+00 .163918E-08 -.125000E-01 .280100E+00
wall id 1478 face -.478354E-02 -.115485E-01 .280100E+00 .163918E-08 -.125000E-01 .260100E+00 .163918E-08 -.125000E-01 .280100E+00
wall id 1479 face .163918E-08 -.125000E-01 .260100E+00 .478354E-02 -.115485E-01 .260100E+00 .478354E-02 -.115485E-01 .280100E+00
wall id 1480 face .163918E-08 -.125000E-01 .280100E+00 .478354E-02 -.115485E-01 .260100E+00 .478354E-02 -.115485E-01 .280100E+00
wall id 1481 face .478354E-02 -.115485E-01 .260100E+00 .883884E-02 -.883883E-02 .260100E+00 .478354E-02 -.115485E-01 .280100E+00
wall id 1482 face .478354E-02 -.115485E-01 .280100E+00 .883884E-02 -.883883E-02 .260100E+00 .478354E-02 -.115485E-01 .280100E+00
wall id 1483 face .883884E-02 -.883883E-02 .260100E+00 .115485E-01 -.478354E-02 .260100E+00 .883884E-02 -.883883E-02 .280100E+00
wall id 1484 face .883884E-02 -.883883E-02 .280100E+00 .115485E-01 -.478354E-02 .260100E+00 .883884E-02 -.883883E-02 .280100E+00
wall id 1485 face .115485E-01 -.478354E-02 .260100E+00 .125000E-01 .218557E-08 .260100E+00 .115485E-01 -.478354E-02 .280100E+00
wall id 1486 face .115485E-01 -.478354E-02 .280100E+00 .125000E-01 .218557E-08 .280100E+00 .115485E-01 -.478354E-02 .280100E+00
wall id 1487 face .125000E-01 .218557E-08 .260100E+00 .115485E-01 .478354E-02 .260100E+00 .125000E-01 .218557E-08 .280100E+00
wall id 1488 face .125000E-01 .218557E-08 .280100E+00 .115485E-01 .478354E-02 .260100E+00 .115485E-01 .478354E-02 .280100E+00

Fz_Calculation.dat
#define FzCalculation

whilestepping

Fz_Sum=0.0
wp=wall_head
loop while wp # null
    if w_id(wp) >= bottom_begin then
        if w_id(wp) <= bottom_end then
            Fz_Sum=Fz_Sum+w_zfob(wp)
        end if
    end if
    wp=w_next(wp)
end_loop
Fz_Bottom= Fz_Sum

Fz_Sum=0.0
wp=wall_head
loop while wp # null
    if w_id(wp) >= cylinder_begin then
        if w_id(wp) <= cylinder_end then
            Fz_Sum=Fz_Sum+w_zfob(wp)
        end if
    end if
    wp=w_next(wp)
end_loop
Fz_Cylinder= Fz_Sum

Fz_Sum=0.0
wp=wall_head
loop while wp # null
    if w_id(wp) >= RodBegin then
        if w_id(wp) <= RodEnd then
            Fz_Sum=Fz_Sum+w_zfob(wp)
        end if
    end if
    wp=w_next(wp)
end_loop
Fz_Top= Fz_Sum
end

Pressure_Calculation.dat
#define PressureCalculation

status= open('WallPressure_Stress_Porosity.fio', I I)
array MessageLine(1)
if UpdateCounter=0 then
  UpdateCounter= UpdateCycles
end_if

command
set fishcall 0 CheckExecution
end_command

end

define CheckExecution

if UpdateCounter=0 then
  UpdateCounter= UpdateCycles
end_if

if UpdateCounter= UpdateCycles then
  UpdateCounter= 0
  ComputePressure
end_if

UpdateCounter= UpdateCounter+ 1
end

define ComputePressure

array CircumForce(10,2)
array Pressure(10,2)
array SumHS(2)

loop iii (1, 10)
  loop jjj (1, 2)
    CircumForce(iii,jjj) = 0.0
    Pressure(iii,jjj) = 0.0
  end_loop
end_loop

loop iii (1, 2)
  SumHS(iii) = 0.0
end_loop

cp = contact_head
loop while cp # null
  EntityB= c_ball2(cp)
  if pointer_type(EntityB)=101 then
    if w_id(EntityB)>= 225 then
      if w_id(EntityB)<= 864 then
        caseof ( w_id(EntityB)=224.1)/(2*32).
          CircumForce(1, 1)= CircumForce(1, 1)+ c_nforce(cp)
          CircumForce(1, 2)= CircumForce(1, 2)+ c_zsforce(cp)
        case 1
          CircumForce(2, 1)= CircumForce(2, 1)+ c_nforce(cp)
          CircumForce(2, 2)= CircumForce(2, 2)+ c_zsforce(cp)
        case 2
          CircumForce(3, 1)= CircumForce(3, 1)+ c_nforce(cp)
          CircumForce(3, 2)= CircumForce(3, 2)+ c_zsforce(cp)
        case 3
          CircumForce(4, 1)= CircumForce(4, 1)+ c_nforce(cp)
          CircumForce(4, 2)= CircumForce(4, 2)+ c_zsforce(cp)
        case 4
          CircumForce(5, 1)= CircumForce(5, 1)+ c_nforce(cp)
          CircumForce(5, 2)= CircumForce(5, 2)+ c_zsforce(cp)
        case 5
          CircumForce(6, 1)= CircumForce(6, 1)+ c_nforce(cp)
          CircumForce(6, 2)= CircumForce(6, 2)+ c_zsforce(cp)
        case 6
          CircumForce(7, 1)= CircumForce(7, 1)+ c_nforce(cp)
          CircumForce(7, 2)= CircumForce(7, 2)+ c_zsforce(cp)
        case 7
          CircumForce(8, 1)= CircumForce(8, 1)+ c_nforce(cp)
          CircumForce(8, 2)= CircumForce(8, 2)+ c_zsforce(cp)
        case 8
          CircumForce(9, 1)= CircumForce(9, 1)+ c_nforce(cp)
          CircumForce(9, 2)= CircumForce(9, 2)+ c_zsforce(cp)
        case 9

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CircumForce(10,1) = CircumForce(10,1) + c_nforce(cp)
CircumForce(10,2) = CircumForce(10,2) + c_zsforce(cp)
end_case
end_if
end_if
end_if

MessageLine(1) = ('Current time=' + time + 'Top force=' + Fz_Top + 'Bottom force=' + Fz_Bottom + 'Friction=' + Fric_Value)
status = write(MessageLine, 1)
end_loop

SigmaH = SumHS(1)/10.0
Tau = SumHS(2)/10.0
FncValue = Tau/SigmaH

Stress_Porosity_Calculation.dat
define StressPorosityCalculation
array Message_Line(1)
if Update_Counter=0 then
  Update_Counter= UpdateCycles
end_if
command
set fishcall 0 Check_Execute
end_command
end
define Check_Execute
if Update_Counter=0 then
  Update_Counter= UpdateCycles
end_if
if Update_Counter= UpdateCycles then
  ComputeStressPorosity
end_if
Update_Counter= Update_Counter+ 1
end
define ComputeStressPorosity
Message_Line(1) = ('Current time=' + time + 'Top force=' + Fz_Top)
status = write(Message_Line, 1)
mp= circ_head
loop while mp # null
  Message_Line(1) = (string(mp) + mp_s11(mp) + mp_s12(mp) + mp_s13(mp) + mp_s21(mp) + mp_s22(mp) + mp_s23(mp) + mp_s31(mp) + mp_s32(mp) + mp_s33(mp) + porous(mp))
  status = write(Message_Line, 1)
mp = m_next(mp)
end_loop
end
Appendix E

Shape functions for a 3-node triangular plate element

E.1 Shape functions

In Chapter 9, the relationship between the displacement field and the nodal displacements is expressed as Eq. (9.7) and reproduced below:

$$\{U\}_{6x1} = [N]_{6x38} \{A\}_{38x1}$$  (9.7)

In Eq. (9.7), the shape function $[N]_{6x38}$ is described in this appendix. As shown in Figure E.1, let a triangular element be defined in the x-y plane by three points $i (x_i, y_i)$, $j (x_j, y_j)$ and $k (x_k, y_k)$ with the origin of the coordinate taken at the centroid $P$, i.e.,

$$\frac{x_i + x_j + x_k}{3} = 0 , \quad \frac{y_i + y_j + y_k}{3} = 0$$  (E.1)

The lengths of side $jk$, side $ki$ and side $ij$ denote respectively by $I_1$, $I_2$ and $I_3$, and are expressed in Eqs. (E.2-E.4). The area of the triangular element, $A_{tr}$, is given by Eq. (E.5).

$$I_1 = \sqrt{(x_k - x_j)^2 + (y_k - y_j)^2}$$  (E.2)
\[ I_2 = \sqrt{(x_i - x_k)^2 + (y_i - y_k)^2} \]  \hspace{1cm} (E.3)

\[ I_3 = \sqrt{(x_j - x_i)^2 + (y_j - y_i)^2} \]  \hspace{1cm} (E.4)

\[ A_{tri} = \frac{1}{2} \begin{vmatrix} x_i & y_i \\ x_j & y_j \\ x_k & y_k \end{vmatrix} \] \hspace{1cm} (E.5)

Let us define area coordinate of a point \( Q \) as follows:

\[ L_1 = \frac{\text{Area} \cdot Qjk}{\text{Area} \cdot ijk}, \quad L_2 = \frac{\text{Area} \cdot Qki}{\text{Area} \cdot ijk}, \quad L_3 = \frac{\text{Area} \cdot Qij}{\text{Area} \cdot ijk} \] \hspace{1cm} (E.6)

**Figure E.1** Local coordinate system and notation

The shape function \([N]_{10\times8}\) can be expressed as Eq. (E.7). It can be seen that the elements in the 6\(^{th}\), 12\(^{th}\) and 18\(^{th}\) columns are set to zero since in-plane rotation is taken to be negligible (\( \theta_z = 0 \)). The other elements are expressed in Eqs. (E.8-E.37).

\[
[N]_{10\times8} = \begin{bmatrix}
N_{13} & 0 & 0 & 0 & 0 & 0 & N_{17} & 0 & 0 & 0 & 0 & N_{33} & 0 & 0 & 0 & 0 \\
0 & N_{22} & 0 & 0 & 0 & 0 & N_{28} & 0 & 0 & 0 & 0 & N_{23} & 0 & 0 & 0 & 0 \\
0 & 0 & N_{33} & N_{34} & N_{35} & 0 & 0 & 0 & N_{39} & N_{310} & N_{311} & 0 & 0 & 0 & 0 & N_{315} & N_{316} & N_{317} & 0 \\
0 & 0 & N_{43} & N_{44} & N_{45} & 0 & 0 & 0 & N_{49} & N_{410} & N_{411} & 0 & 0 & 0 & N_{415} & N_{416} & N_{417} & 0 \\
0 & 0 & N_{53} & N_{54} & N_{55} & 0 & 0 & 0 & N_{59} & N_{510} & N_{511} & 0 & 0 & 0 & N_{515} & N_{516} & N_{517} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{bmatrix} \] \hspace{1cm} (E.7)
\[ N_{11} = N_{22} = \frac{(a_1 + b_1x + c_1y)}{2A_{\text{tri}}} \]  

(E.8)

\[ N_{17} = N_{28} = \frac{(a_2 + b_2x + c_2y)}{2A_{\text{tri}}} \]  

(E.9)

\[ N_{1,13} = N_{2,14} = \frac{(a_3 + b_3x + c_3y)}{2A_{\text{tri}}} \]  

(E.10)

\[ N_{3,3} = P_1 - P_4 + P_6 + 2(P_7 - P_9) \]  

(E.11)

\[ N_{3,9} = P_2 - P_5 + P_4 + 2(P_8 - P_7) \]  

(E.12)

\[ N_{3,15} = P_3 - P_6 + P_5 + 2(P_9 - P_8) \]  

(E.13)

\[ N_{3,4} = -b_2(P_9 - P_6) + b_1P_7 \]  

(E.14)

\[ N_{3,10} = -b_3(P_7 - P_4) + b_1P_8 \]  

(E.15)

\[ N_{3,16} = -b_1(P_8 - P_5) + b_2P_9 \]  

(E.16)

\[ N_{3,5} = -c_2(P_9 - P_6) + c_3P_7 \]  

(E.17)

\[ N_{3,11} = -c_3(P_7 - P_4) + c_2P_8 \]  

(E.18)

\[ N_{3,17} = -c_1(P_8 - P_5) + c_3P_8 \]  

(E.19)

\[ N_{4,3} = \frac{\partial N_{33}}{\partial y} = \frac{\frac{c_1 \partial N_{33}}{\partial L_1} + c_2 \frac{\partial N_{33}}{\partial L_2} + c_3 \frac{\partial N_{33}}{\partial L_3}}{2A_{\text{tri}}} \]  

(E.20)

\[ N_{4,9} = \frac{\partial N_{39}}{\partial y} = \frac{\frac{c_1 \partial N_{39}}{\partial L_1} + c_2 \frac{\partial N_{39}}{\partial L_2} + c_3 \frac{\partial N_{39}}{\partial L_3}}{2A_{\text{tri}}} \]  

(E.21)

\[ N_{4,15} = \frac{\partial N_{3,15}}{\partial y} = \frac{\frac{c_1 \partial N_{3,15}}{\partial L_1} + c_2 \frac{\partial N_{3,15}}{\partial L_2} + c_3 \frac{\partial N_{3,15}}{\partial L_3}}{2A_{\text{tri}}} \]  

(E.22)

\[ N_{4,4} = \frac{\partial N_{34}}{\partial y} = \frac{\frac{c_1 \partial N_{34}}{\partial L_1} + c_2 \frac{\partial N_{34}}{\partial L_2} + c_3 \frac{\partial N_{34}}{\partial L_3}}{2A_{\text{tri}}} \]  

(E.23)

\[ N_{4,10} = \frac{\partial N_{3,10}}{\partial y} = \frac{\frac{c_1 \partial N_{3,10}}{\partial L_1} + c_2 \frac{\partial N_{3,10}}{\partial L_2} + c_3 \frac{\partial N_{3,10}}{\partial L_3}}{2A_{\text{tri}}} \]  

(E.24)
\[
N_{4,16} = \frac{\partial N_{3,16}}{\partial y} = \frac{c_1 \frac{\partial N_{3,16}}{\partial L_1} + c_2 \frac{\partial N_{3,16}}{\partial L_2} + c_3 \frac{\partial N_{3,16}}{\partial L_3}}{2A_{tri}} \quad (E.25)
\]
\[
N_{4,5} = \frac{\partial N_{3,15}}{\partial y} = \frac{c_1 \frac{\partial N_{3,15}}{\partial L_1} + c_2 \frac{\partial N_{3,15}}{\partial L_2} + c_3 \frac{\partial N_{3,15}}{\partial L_3}}{2A_{tri}} \quad (E.26)
\]
\[
N_{4,11} = \frac{\partial N_{3,11}}{\partial y} = \frac{c_1 \frac{\partial N_{3,11}}{\partial L_1} + c_2 \frac{\partial N_{3,11}}{\partial L_2} + c_3 \frac{\partial N_{3,11}}{\partial L_3}}{2A_{tri}} \quad (E.27)
\]
\[
N_{4,17} = \frac{\partial N_{3,17}}{\partial y} = \frac{c_1 \frac{\partial N_{3,17}}{\partial L_1} + c_2 \frac{\partial N_{3,17}}{\partial L_2} + c_3 \frac{\partial N_{3,17}}{\partial L_3}}{2A_{tri}} \quad (E.28)
\]
\[
N_{5,3} = -\frac{\partial N_{33}}{\partial x} = -\frac{b_1 \frac{\partial N_{33}}{\partial L_1} + b_2 \frac{\partial N_{33}}{\partial L_2} + b_3 \frac{\partial N_{33}}{\partial L_3}}{2A_{tri}} \quad (E.29)
\]
\[
N_{5,9} = -\frac{\partial N_{39}}{\partial x} = -\frac{b_1 \frac{\partial N_{39}}{\partial L_1} + b_2 \frac{\partial N_{39}}{\partial L_2} + b_3 \frac{\partial N_{39}}{\partial L_3}}{2A_{tri}} \quad (E.30)
\]
\[
N_{5,15} = -\frac{\partial N_{3,15}}{\partial x} = -\frac{b_1 \frac{\partial N_{3,15}}{\partial L_1} + b_2 \frac{\partial N_{3,15}}{\partial L_2} + b_3 \frac{\partial N_{3,15}}{\partial L_3}}{2A_{tri}} \quad (E.31)
\]
\[
N_{5,4} = -\frac{\partial N_{34}}{\partial x} = -\frac{b_1 \frac{\partial N_{34}}{\partial L_1} + b_2 \frac{\partial N_{34}}{\partial L_2} + b_3 \frac{\partial N_{34}}{\partial L_3}}{2A_{tri}} \quad (E.32)
\]
\[
N_{5,10} = -\frac{\partial N_{3,10}}{\partial x} = -\frac{b_1 \frac{\partial N_{3,10}}{\partial L_1} + b_2 \frac{\partial N_{3,10}}{\partial L_2} + b_3 \frac{\partial N_{3,10}}{\partial L_3}}{2A_{tri}} \quad (E.33)
\]
\[
N_{5,16} = -\frac{\partial N_{3,16}}{\partial x} = -\frac{b_1 \frac{\partial N_{3,16}}{\partial L_1} + b_2 \frac{\partial N_{3,16}}{\partial L_2} + b_3 \frac{\partial N_{3,16}}{\partial L_3}}{2A_{tri}} \quad (E.34)
\]
\[
N_{5,5} = -\frac{\partial N_{35}}{\partial x} = -\frac{b_1 \frac{\partial N_{35}}{\partial L_1} + b_2 \frac{\partial N_{35}}{\partial L_2} + b_3 \frac{\partial N_{35}}{\partial L_3}}{2A_{tri}} \quad (E.35)
\]
\[
N_{5,11} = -\frac{\partial N_{3,11}}{\partial x} = -\frac{b_1 \frac{\partial N_{3,11}}{\partial L_1} + b_2 \frac{\partial N_{3,11}}{\partial L_2} + b_3 \frac{\partial N_{3,11}}{\partial L_3}}{2A_{tri}} \quad (E.36)
\]
\[ N_{5,17} = -\frac{\partial N_{3,17}}{\partial x} = -\frac{b_1 \frac{\partial N_{3,17}}{\partial L_1} + b_2 \frac{\partial N_{3,17}}{\partial L_2} + b_3 \frac{\partial N_{3,17}}{\partial L_3}}{2A_{tri}} \quad (E.37) \]

The symbols \( i.e. a_1, a_2, a_3, b_1, b_2, b_3, c_1, c_2, c_3, P_1, P_2, P_3, P_4, P_5, P_6, P_7, P_8, P_9, \mu_1, \mu_2, \mu_3 \) in Eqs. (E.8-E.37) are defined as follows:

\[ a_1 = x_j y_k - x_k y_j, \quad a_2 = x_k y_i - x_i y_k, \quad a_3 = x_i y_j - x_j y_i \quad (E.38) \]

\[ b_1 = y_j - y_k, \quad b_2 = y_k - y_i, \quad b_3 = y_i - y_j \quad (E.39) \]

\[ c_1 = x_k - x_j, \quad c_2 = x_i - x_k, \quad c_3 = x_j - x_i \quad (E.40) \]

\[ P_1 = L_1 \quad (E.41) \]

\[ P_2 = L_2 \quad (E.42) \]

\[ P_3 = L_3 \quad (E.43) \]

\[ P_4 = L_1 L_2 \quad (E.44) \]

\[ P_5 = L_2 L_3 \quad (E.45) \]

\[ P_6 = L_3 L_1 \quad (E.46) \]

\[ P_7 = L_1^2 L_2 + 0.5 L_4 L_2 L_3 [3(1 - \mu_3) L_1 + (1 + 3 \mu_3) (L_3 - L_2)] \quad (E.47) \]

\[ P_8 = L_2^2 L_3 + 0.5 L_4 L_2 L_3 [3(1 - \mu_1) L_2 + (1 + 3 \mu_1) (L_1 - L_3)] \quad (E.48) \]

\[ P_9 = L_3^2 L_1 + 0.5 L_4 L_2 L_3 [3(1 - \mu_2) L_3 + (1 + 3 \mu_2) (L_2 - L_1)] \quad (E.49) \]

\[ \mu_1 = \frac{(I_3^2 - I_2^2)}{I_1^2}, \quad \mu_2 = \frac{(I_1^2 - I_3^2)}{I_2^2}, \quad \mu_3 = \frac{(I_2^2 - I_1^2)}{I_3^2} \quad (E.50) \]
E.2 ABAQUS input file

ABAQUS input files were used to calculate the stress distribution of the cylinder resulting from DEM boundary forces. A typical ABAQUS input file is listed below.

*HEADING
Input file for modelling confined compression glass beads.

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***************ELEMENT DESIGNATION************************************************************

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147, 66, 67, 226
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*NSET,NSET=BOUND,GENDRATE

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**SECTIONAL PROPERTIES**

*SHELL,SECT=TRIANGLE,MatE=ACRYLIC

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**MATERIAL PROPERTIES**

*MATERIAL,NAME=ACRYLIC

*ELASTIC

2.90E+9,0.35

**BOUNDARY CONDITIONS**

*BOUNDARY

BOUND,ENCASSTRE

**RESTART FILE**

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*CLOAD

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Appendix F

Fortran program for solving Eq. (5.14)

The following Fortran program was coded to obtain the solution for Eq. (5.14) using the bisection method. This program also was used to calculate the Young's modulus of a single grain, $a$ and $b$ in Figure 5.5.

```fortran
program HERTZ_Paper
  use msimsl
  call input
  call solver
  call output
  end

  subroutine input
    implicit none
    integer ENDS, max_case
    parameter (ENDS=2, max_case=500)
    integer i
    integer INCREMENT, n_case
    double precision rb, rs, mu
    double precision FORCE(max_case), DISP(max_case)
    double precision AB(ENDS)
    double precision beta
    common /a/ AB, INCREMENT
    common /b/ beta
    common /d/ rb, rs, mu
    common /e/ FORCE, DISP
    common /f/ n_case
  end subroutine input
```

318
C  open (11, file= 'HERTZ_Paper_INPUT.DAT')
open (12, file= 'HERTZ_Paper_OUTPUT.DAT')
C
write(*,*) 'please input the radii of curvature: R1' and R1
read(11,*) rb, rs
C  write(*,*) 'please input the Poisson's ratio'
read(11,*) mu
C  write(*,*) 'please input two ends of the interval'
do i=1,ENDS
   read(11,*) AB(i)
end do
C  write(*,*) 'please input the number of increment'
read(11,*) INCREMENT
C  write(*,*) 'please input the case number'
read(11,*) n_case
C  write(*,*) 'please input the force and displacement'
do i=1, n_case
   read(11,*) DISP(i), FORCE(i)
end do
C
beta=(rb-rs)/(rb+rs)
C
return
end
C
C subroutine solver
implicit none
integer ENDS
parameter (ENDS=2)
integer MAXFN
integer INCREMENT
integer ii
integer IN
double precision AB(ENDS)
double precision DET
double precision ERRABS, ERRREL
double precision step, AA, BB
common /a/ AB, INCREMENT
common /c/ BB, MAXFN
external DET, DZBREN, IN
C
C ERRABS = 1.0E-10
ERRREL = 1.0E-10
MAXFN = 100
C
step=(AB(2)-AB(1))/real(INCREMENT)
do ii=1, INCREMENT
   AA=AB(ii-1)+(ii-1)*step
   BB=AA+step
   if (DET(AA),DET(BB)) .eq. -1) then
      To find the zero
      CALL DZBREN (DET, ERRABS, ERRREL, AA, BB, MAXFN)
      go to 10
   end if
C

subroutine output
  implicit none
  integer max_case, n_case
  parameter (max_case=500)
  integer MAXFN, i
  double precision BB
  double precision rb, rs, mu
  double precision FORCE(max_case), DISP(max_case)
  double precision DELK, DELE
  double precision KK, EE, stiff
  double precision E
  double precision PI
  double precision Radiusa, Radiusb
  parameter (PI=3.14159265359)
  common /c// BB, MAXFN
  common /d// rb, rs, mu
  common /e// FORCE, DISP
  common /f// n_case
  external DELK, DELE

  do i=1, n_case
    KK=DELK(BB).
    EE=DELE(BB).
    stiff=sqrt(4.0*EE*DISP(i)**3
      &/(9.0*FORCE(i)*FORCE(i)*0.5*(1.0/rb+1.0/rs)*(1-BB)*KK**3))
    E=(1.0-mu*mu)/(PI*stiff)
    Radiusa=(3.0*DISP(i)*stiff*EE/(1.0/rb+1.0/rs)/(1.0-BB))**(1.0/3.0)
    Radiusb=Radiusa*sqrt(1.0-BB)
    write(12,101) MAXFN, BB, E, Radiusa, Radiusb
  end do
  101 format(1x,i6,lx,e16.6,1x,e16.6,1x,e16.6,1x,e16.6)
  return
end
double precision DELK, DELE
double precision KK, EE
double precision beta
common /b/ beta
external DELk, DELE

KK=DELK(Y)
EE=DELE(Y)
DET=2.0*(KK-EE)*(1.0-Y)-(1.0-beta)*Y*EE

return
derived

integer function IN(FAA,FBB)
implicit none
double precision FAA,FBB

if (FAA .gt. 0.) then
  if (FBB .lt. 0.) then
    IN=-1
  else
    IN=+1
  end if
else
  if (FBB .gt. 0.) then
    IN=-1
  else
    IN=+1
  end if
end if

return
derived
Appendix G

Publications
MEASUREMENT OF MECHANICAL PROPERTIES OF AGRICULTURAL GRAINS FOR DE MODELS
Y.C. Chung¹, J.Y. Ooi² and J. Favier³

ABSTRACT

The Discrete Element (DE) method has been used extensively in recent times to study the behaviour of granular systems. The paper describes the first phase of a project to develop DE models for representing agricultural grains with a level of accuracy sufficient to represent the dynamic behaviour of these grains in agricultural equipment. In the project, both novel and standard measurements of relevant mechanical and geometrical properties of grains for use in DE simulations will be made. A set of simple physical experiments including filling of a container, vertical compression of the grains in a container and flow of the grains of a container will be conducted. The shape and size of each grain type will be represented using a multi-sphere particle model, allowing the non-spherical shape of the grains to be adequately modelled. DE simulations using these multi-sphere particles will be conducted and a comparison made between the simulated and the measured response. In this paper the methods used to determine some mechanical parameters and first results from the experiments will be presented.

Keywords: discrete element, non-spherical particle, agricultural grains, corn, mechanical property, compression test, sliding test, drop test

INTRODUCTION

There are many processes in the agricultural industry in which the grains undergo a variety of stress and deformation regimes. These include seeding, harvesting, conveying, transporting and storing, to name a few. A better modelling and understanding of the flow behaviour of agricultural grains should lead to improved methods for these handling processes. It is proposed that the Discrete Element (DE) computer simulations be used to model such processes. This paper describes the first phase of a project to develop DE models for representing agricultural grains with a level of accuracy sufficient to represent the dynamic behaviour of these grains in agricultural equipment. In the project, relevant mechanical and geometrical properties of single grain and grain bulks will be measured and the values used to calibrate associated DE models of

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grain behaviour. These models will then be used to validate 3D DE simulations of chosen agricultural grains in controlled experiments at the micro (particle) and macro (bulk) scales.

In order to acquire meaningful results, it is essential that the parameters involved in the DE model be carefully determined. These parameters include the mechanical and geometric properties of the grains: Young's modulus, Poisson's ratio, friction coefficient, coefficient of restitution, mass, and geometric shape parameters. The laboratory tests devised to measure these parameters consisted of single particle compression test, sliding friction test, Jenike shear test and drop test with 3D laser scanning technique. This paper describes primarily the first phase of the project on the measurements of material parameters, which provide a valuable database of measured mechanical and geometric properties of corn grains. The methodology developed for determining these parameters can be applied to other spherical and non-spherical particles.

These measured parameters are being used in DE simulations of several calibration experiments using the DE modelling software, provided by DEM Solutions Ltd. These calibration experiments comprise filling of a container, vertical confined compression test, silo discharge test, and penetration test of a cylindrical rod into a granular medium. Three dimensional DE simulations of these experiments will be performed, with careful consideration of the geometry and kinematics of boundary surfaces and the initial positions, orientations and kinematics of the grains. Overlapping spheres (Multi-Sphere method) will be used to represent the shape of the agricultural grain in these 3D simulations. The comparison between the simulated and measured behaviour will provide some validation on the number of spheres required to adequately account for the particle shape. The initial progress on these calibration experiments and DE simulations is discussed. The detailed theoretical considerations and experimental results for each proposed experimental method will be provided at a later date.

DETERMINATION OF PARAMETERS FOR DE SIMULATIONS

Several apparatuses have been developed and used to determine the parameters required for DE simulations. All six types of corn grains, which are labelled A, B, C, D, E and F respectively, were tested. Some results of measurements are described below.

Young's modulus and Poisson's ratio:

The Hertzian contact theory has widely been used to determine the modulus of elasticity for various agricultural grains (Shelef and Mohsenin, 1969; Amold and Roberts, 1969; Misra and Young, 1981; Jindal and Techasena, 1985). This determination is based on fitting the Hertzian model to the force-displacement data from the single particle compression test and assuming a value of the Poisson's ratio, as described in the ASAE Standard (1996).

In the first instance, the ASAE Standard single particle compression test using a spherical indenter was carried out to deduce the elastic properties for corn grains. However, it has been observed that when the particle is not very flat in the region of contact, the indenter slips and bents during the test. In these cases, the contact area is no longer circular or elliptical and the line of the applied load is also no longer vertical. Thus, the indenter method is not suitable for particles that are not sufficiently flat. To overcome these, it is proposed that a vertical compression of the particle between two rigid platens is conducted to evaluate the mechanical properties of the smaller grains in combination with a 3D laser scanning technique (3D Scanners Ltd., 1998). The 3D laser scanner was used to capture the three-dimensional surface geometry of
individual grains, so that the radii of curvature at the point of contact can be accurately
determined. This improved method for determining the Young's modulus for agricultural grains
was developed by first reviewing a set of transcendental equations (Hertz, 1896) which Hertz
derived for more general cases; secondly, providing a simple approach to solve these equations,
and finally evaluating the effect of the assumed value of the Poisson's ratio on the calculation
(instead of simply assuming a value).

The 3D laser scanner was used to capture the three-dimensional surface geometry of
individual grains. Figures 1 and 2 show typical X-Z and Y-Z plane curves for a single grain
(corn type D), which intersect at the point of contact (the highest point). The radii of curvature in
the mutually perpendicular planes can be determined from the scanned data and used for
determining the Young's modulus.

![Curve in X-Z](image)

![Curve in Y-Z](image)

**FIG. 1. Curve in X-Z plane (corn D)**

**FIG. 2 Curve in Y-Z plane (corn D)**

The single particle compression tests were carried out in an Instron machine (Model 4500
Testing System). The germ-side surface of each kernel was lightly sanded (in order that it is very
flat and the deformation on this surface can be assumed to be negligible during the compression)
and the kernels were glued, germ-side down, to a flat metal plate. The vertical load was applied to
the surface of the kernel on the horny endosperm. Both test methods, the ASAE Standard indenter
method and this proposed method of compression between rigid platens, were performed. Three
grains for each corn type were tested. The results for both methods are given in Table 1.
TABLE 1. Young’s moduli for six types of corn grains

<table>
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<tr>
<th>Corn type</th>
<th>Mean Young’s modulus (MPa)</th>
<th>Mean Young’s modulus (MPa)</th>
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<td>(based on the ASAE indenter method)</td>
<td>(based on the proposed method)</td>
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<tr>
<td>B</td>
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<td>2320</td>
</tr>
<tr>
<td>C</td>
<td>-</td>
<td>1330</td>
</tr>
<tr>
<td>D</td>
<td>-</td>
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</tr>
<tr>
<td>E</td>
<td>-</td>
<td>2160</td>
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<tr>
<td>F</td>
<td>1040</td>
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The range of the Young’s moduli for the six types of corn grains based on the proposed rigid platen compression method is 1040-2320 MPa with a mean of 1660 MPa and a coefficient of variation of 31%. A reference value of the Young’s modulus for yellow dent hybrid corn (WF9MST×H71) (Oh43RF×B37RF) is given as 2030 MPa in the ASAE Standard (1996). This value is comparable with the measurements obtained in this study. The average Young’s moduli for corn A and F based on the ASAE method are 900 and 1040 MPa respectively, whilst those based on the proposed method are 1320 and 1040 MPa. The result obtained from the ASAE method thus matches that from the proposed method for corn F but differs significantly for corn A. The ASAE method is not suitable for corn grains such as B, C, D and E because they are not flat, thus causing the spherical indenter to slip and bent during the test.

In the study by Shelef and Mohsenin (1969), the upper surface of kernels was finely sanded by means of a specially built mechanical sander to make the upper surface flat. The exposed area consisted of horny endosperm, varying in depth, and floury endosperm at the dent. However, this process may disturb the stiffness and strength of corn grains. In contrast, the upper surface of kernels was not tempered with in the proposed rigid platen compression method.

Friction coefficient:

Many researchers have attempted to measure the friction coefficient. For example, Lorenz et al (1997) calculated dynamic inter-particle friction coefficients for different types of material, such as polystyrene, stainless steel, acrylic and glass beads performing a binary collision experiment based on the Walton’s impact model. O’Sullivan et al. (2003) presented a modified four-ball test to obtain static inter-particle friction coefficient for steel balls and conducted tilt tests to determine static friction coefficients between the steel balls and the boundary surface. However, the above research is limited to spherical or nearly spherical particles and may not be suitable for irregularly shaped particles, like corn grains and other cereal grains. The literature on the measurement of friction coefficient for irregularly shaped particles is extremely limited.

In the present study, the static particle-surface friction coefficients for irregularly shaped particles were estimated from a simple sliding test. The bulk friction coefficients were measured using the Jenike shear test (IChE, 1989). The inter-particle bulk friction coefficient will be measured using the internal friction test, whilst the wall friction test will be used to determine the particle-surface friction coefficients.

Three samples for each corn type were tested in the sliding friction test. Each test was
repeated three times. Three corn grains are selected randomly for each test. The germ-side surface of each kernel is sanded until all three have the same height. To make sure of this, they are put on a horizontal surface, the test plate is put on top of the three corn grains, and the level of the test plate checked using a spirit level. After this verification, three grains are then glued, horny endosperm-side up, on the horizontal base plate. The test plate is not glued but placed on top of the three grains and the level is checked again to ensure that it is horizontal. During the test, the inclination of the base plate is gradually increased using a jack, until relative sliding between the grains and the test plate occurs. The angle ($\theta$) of the inclination of the base plate at this instant is measured. The static particle-surface friction coefficient ($\mu$) can be determined from 

$$\mu = \tan \theta.$$ 

Two different surfaces were tested: steel and aluminium. Two test plates were provided by a silo manufacturer. Figure 3 shows the friction coefficients obtained for three samples of corn A. The data obtained for the remaining corn types are quite similar to the one shown here. The results for the six types of corn grains with the aluminium plate and the stainless steel plate are shown in Tables 2 (a) and (b) respectively. It can be seen that the variation coefficient (ratio of standard deviation to mean) for each test is less than 10% and the variation coefficient for each corn is also less than 10%. The friction coefficients for the six corn types with the aluminium test plate vary from 0.226 to 0.276, whilst the corresponding range for the stainless steel test plate is 0.476-0.596. These values are all within the range reported by Kemnitz (1975). It should also be noted that the higher friction coefficient measured for the stainless steel plate in this study might be due to the features of this particular test plate. The stainless steel test plate was obtained from a silo manufacturer. Visual inspection reveals unidirectionally brushed stripes on the plate. The friction tests were conducted with the stripes perpendicular to the direction of motion. This may be the reason why the friction coefficients for the stainless steel plate are higher.

![FIG. 3 Friction coefficient measurements for Corn A](image-url)
### TABLE 2. Friction coefficients for the six corn types

<table>
<thead>
<tr>
<th>Corn</th>
<th>Friction coefficient</th>
<th>Coefficient of variation (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0.226</td>
<td>5.5</td>
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<tr>
<td>B</td>
<td>0.249</td>
<td>8.5</td>
</tr>
<tr>
<td>C</td>
<td>0.256</td>
<td>2.9</td>
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<tr>
<td>D</td>
<td>0.276</td>
<td>9.9</td>
</tr>
<tr>
<td>E</td>
<td>0.263</td>
<td>3.0</td>
</tr>
<tr>
<td>F</td>
<td>0.254</td>
<td>5.6</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Corn</th>
<th>Friction coefficient</th>
<th>Coefficient of variation (%)</th>
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</thead>
<tbody>
<tr>
<td>A</td>
<td>0.519</td>
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<td>B</td>
<td>0.476</td>
<td>5.8</td>
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<tr>
<td>C</td>
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<tr>
<td>E</td>
<td>0.596</td>
<td>4.4</td>
</tr>
<tr>
<td>F</td>
<td>0.553</td>
<td>3.6</td>
</tr>
</tbody>
</table>

**Coefficient of restitution:**

Most real particles, for example, agricultural grains, are not spheres. The literature concerning the coefficient of restitution for irregularly shaped particles is very limited. LoCurto et al. (1997) determined the energy restitution coefficient for soybeans by conducting a simple drop test. In their experiments, only soybeans which rebounded with minimal rotation and with trajectories within \((88.6° - 91.4°)\) range (inclination to the plate i.e. nearly vertical) were selected. This is because it is possible for a proportion of these somewhat spherical soybeans to rebound nearly vertically so that the energy can be translated to the height of rebound. However, it is difficult to apply such test for irregularly shaped particles, since they will rebound randomly and very possibly with significant rotation. To date, only Yang and Schrock (1994) carried out a 3-D analysis to acquire the normal and resultant restitution coefficients for irregularly shaped particles such as wheat, soybean, cheat, and goatgrass similarly using the drop test method. However they did not measure the rotational velocity after impact in their tests. The energy restitution coefficient was thus impossible to determine, as the rotational kinetic energy cannot be evaluated.

In the present study, the drop test is extended to provide a methodology to evaluate the energy restitution coefficient for any irregularly shaped particles. The method will also give the normal, tangential and resultant restitution coefficients. The rebounding linear and angular velocities at any instant is determined from the images taken using a high-speed camera. The 3D laser scanner is used to capture the three-dimensional surface geometry of the irregularly shaped test objects. The scanned data will be processed to determine the mass moments and products of inertia at any instant. The rotational kinetic energy together with translational kinetic energy can be evaluated, and the energy restitution coefficient can then be calculated. The results should facilitate the development of the contact model for irregularly shaped particles in DEM, and provide data for calibration and simple validation.
Calibration experiments

The confined compression test (Masroor et al, 1987) is designed to investigate the mechanical response of a granular material under vertical loading and the load transfer to the containing walls. A load is applied to the grain bulk contained in a thin-walled cylinder through a piston driven by an INSTRON machine. The applied load and vertical displacement are measured using a proving ring and an LVDT displacement transducer respectively. The forces transmitted to the walls is measured using strain gauges fixed to the cylinder wall in both circumferential and axial directions. The vertical force transmitted to the bottom piston is measured by the bottom load cell. Preliminary experiments have been carried out using glass beads with a diameter of 10 mm. The number of glass beads is approximately 3590. Figure 4 shows the vertical stress and vertical strain relationship, indicating the increasing stiffness in the system as loading increases. The load transfer to the containing walls is investigated by studying the stress ratio (ratio of horizontal stress to vertical stress) and mobilized wall friction coefficient (ratio of shear stress to horizontal stress on the wall) during vertical loading, as shown in Figure 5. It can be seen that the mobilized wall friction swiftly reached a relatively constant value of 0.18. The stress ratio, which is similar to the lateral pressure ratio in Janssen theory (Ooi and Rotter, 1990), increases swiftly and then stays between 0.7–0.8. It would be very interesting to see whether DE simulations could match these observations.

![FIG. 4 Vertical stress and strain relation](image)

![FIG. 5 Stress ratio and wall friction coefficient against the load](image)

CONCLUSIONS

The first stage of the project to develop DE models to simulate dynamic behaviour of grains in agricultural equipment has been described. Several apparatuses have been developed and used to determine the parameters required for DE simulations. The proposed rigid platen compression method together with the 3D laser technique has been shown to give a sound measurement of elastic modulus, which is applicable to any irregularly shaped agricultural grains, regardless of size and shape. The sliding friction test has been shown to be stable and reproducible, again applicable to any irregularly shaped agricultural grains. The friction
coefficient appears to be dominated by the type of metal plate, with the different types of corn grains having only small effect.

In addition, several calibration experiments have been carefully devised and will be used to calibrate and validate the DE models in this project. Some results of the confined compression test have been presented, revealing the load transfer to the containing walls. DE simulations of these calibration experiments are underway and the results will be compared with the experimental observations.

ACKNOWLEDGMENTS

The authors would like to acknowledge Deere & Company, DEM Solutions Ltd. and School of Engineering & Electronics at the University of Edinburgh for funding this research. The authors are very grateful to Dr Carol Plouffe for his advice and discussion about this project.

REFERENCES


EXPERIMENTAL MEASUREMENT AND DISCRETE ELEMENT MODELLING OF A DENSE GRANULAR MEDIUM UNDER LOADING

Y.C. Chung, Institute for Infrastructure & Environment, University of Edinburgh  
J.Y. Ooi, Institute for Infrastructure & Environment, University of Edinburgh

ABSTRACT

In many scientific and industrial applications involving granular solids, the Discrete Element Method (DEM) has been used to investigate the response of the granular system. However, the majority of the numerical simulations were often not validated or compared with experimental results. This paper describes DEM simulations of two laboratory experiments conducted on a densely packed granular medium. The results of the simulations and the experiments were compared and discussed. A comparison with an analytical solution was also made, giving reasonable agreement. The investigation of particle stiffness suggests that whilst it is important to use the correct particle stiffness parameter when attempting to predict the deformation response of a granular system, it may not be so important for producing satisfactory prediction of the force transmission in a dense quasi-static system.

INTRODUCTION

Many of the materials handled by industry each year are of a granular or particulate nature. In recent years, the Discrete Element Method (DEM) [1] has been used extensively to investigate the behaviour of granular solids subjected to a variety of loading conditions. However, the majority of the numerical simulations were often not validated or compared with experimental results. There is thus a need to verify if DEM is capable of producing quantitative predictions and to investigate the relative importance of the DEM input parameters for producing satisfactory predictions.

This paper describes the experiments and DEM simulations of a densely packed granular medium subjected to compression and penetration. The experimental setup consists of an instrumented Perspex cylinder filled with granular solids. The first experiment was to compress the solid vertically under predominantly Ko (zero lateral deformation) condition and the second was to insert a cylindrical rod into the granular medium. The mechanical response of the granular system and the load transfer to the containing walls, the bottom platen and the rod were observed.

Glass beads were studied. The required mechanical and geometrical properties for glass beads were measured carefully for use in the corresponding DEM simulations. The simulations are performed using the EDEM software from DEM Solutions Limited. An extensive study exploring the sensitivity of DEM prediction to the key input parameters is underway. This paper describes some of the comparison between simulation and experiment. The results suggest that whilst it is important to use the correct particle stiffness parameter when attempting to predict the deformation response of a granular system, it may not be so important for producing satisfactory prediction of the force transmission in a dense quasi-static system.

CALIBRATION EXPERIMENTS

The Ko compression test [2], as shown in Fig.1, was designed to investigate the mechanical response of a granular material under vertical loading and the load transfer to the containing walls. A load was applied to the grain bulk contained in a thin-walled cylinder through a piston driven by an INSTRON machine. The applied load and vertical displacement were measured using a proving ring and an LVDT displacement transducer respectively. The force transmitted to the walls was measured using strain gauges fixed to the cylinder walls in both circumferential and axial directions. The vertical force transmitted to the bottom piston was measured by the bottom load cell.

The penetration test was designed to evaluate the resistance of grain bulk to penetration of a moving object as well as dynamic force transmission to a contact surface. The experimental design is depicted in Fig.2. The force and displacement of a rod were monitored using an INSTRON machine as the rod was pushed into grain bulk at constant displacement rate.
DEM SIMULATIONS

Three-dimensional DEM simulations were performed using EDEM software. The Hertz-Mindlin contact model with no slip [3] was used to model the contact between particles and between particles and boundary. This model involves a spring and a damper in the normal direction (n) and a spring and a damper limited by sliding friction in the tangential direction (t), as shown in Fig. 3. The key input parameters include the Young's modulus (or shear modulus), Poisson's ratio, friction coefficient, and coefficient of restitution.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td>2530</td>
<td>kg/m³</td>
</tr>
<tr>
<td>Diameter</td>
<td>10 +/- 0.5 (tolerance)</td>
<td>mm</td>
</tr>
<tr>
<td>Young's modulus</td>
<td>41</td>
<td>GPa</td>
</tr>
<tr>
<td>Poisson's ratio</td>
<td>0.22</td>
<td></td>
</tr>
<tr>
<td>Friction coefficient</td>
<td>0.24</td>
<td></td>
</tr>
<tr>
<td>Restitution Coefficient</td>
<td>0.79</td>
<td></td>
</tr>
</tbody>
</table>

Figure 3: Spring and dashpot contact model

Input parameters for glass beads are listed in Table 1. The Young's modulus was determined from the single particle compression test. A sliding test apparatus was devised to measure the static particle-surface friction coefficient. A drop test apparatus has been built to determine the coefficient of restitution. More details of the above tests can be found in [4, 5].

The numerical samples were prepared by filling a cylindrical container (diameter=145mm, length=300mm) with approximately 3590 glass beads. At the beginning, these glass beads were positioned as shown in Fig. 4 with initial velocity of 2.56 m/s in order to save computational time and then they were allowed to fall under gravity. The initial velocity corresponds to the drop height of 335 mm in the experiments. These glass beads were deemed to have settled down when the kinetic energy of the system approached zero (<10^-8 J). The \( K_0 \) compression was simulated by adding a top platen moving at a displacement rate of 50 mm/min, as shown in Fig. 5. The rod penetration was simulated by adding a rod moving at a displacement rate of 50 mm/min, as shown in Fig. 6.
**K₀ COMPRESSION TEST: RESULTS AND DISCUSSION**

The first set of experiments was conducted using glass beads with a mean diameter of 10 mm. The number of glass beads was approximately 3590. In the experiment, the displacement rate of the top platen was set to 1.5 mm/min. Fig. 7(a) shows the load-displacement relationship, indicating increasing stiffness as vertical load increases. The initial stage of loading was sensitive to the initial packing for each experiment. However, the load-displacement responses at later stages were largely parallel, indicating repeatable loading response for the system. Fig. 7(b) shows the typical force transmission onto the bottom platen and cylindrical walls during compression.

DEM simulations were first conducted with reduced shear modulus in order to reduce computational effort. Three cases were run with particle shear modulus set at $10^{-2} \text{G}$, $10^{-3} \text{G}$ and $10^{-4} \text{G}$, where $\text{G}$ is the measured shear modulus of individual glass beads. The effect of particle stiffness in DEM calculations was explored to evaluate the sensitivity of the input parameter to produce realistic predictions. Fig. 8 shows the load-displacement curves for the three cases. As expected, the bigger the shear modulus, the higher the stiffness in the load-displacement curves. The results are currently being analysed further and further progress will be reported in due course.

Fig. 9 compares the force transfer into the bottom platen and cylindrical walls as a function of the applied force on the top platen. It indicates that as the shear modulus of the particles was reduced from $0.01 \text{G}$ to $0.0001 \text{G}$, the share of the force carried by the cylindrical walls increased slightly. This suggests that for a confined quasi-static system, reduction of particle stiffness by a few orders may have only a small effect on the load transfer mechanism. This plot also compares the numerical results with those from experiments, indicating that the DE predictions match the experimental results reasonably well.
ROD PENETRATION TEST: RESULTS AND DISCUSSION

Fig. 13 shows the load-displacement response for the rod penetration into glass beads. In the experiment, the displacement rate of the steel rod was set to 50 mm/min. The measured force fluctuated significantly during penetration but the average trend for the three tests is repeatable. Shown in Fig. 14 are the DEM results, conducted with a reduced shear modulus at 0.01G and increased density \( \rho \) at 1000\( \rho \) to reduce computational effort. This initial simulation result appears to show similar trend to the experiments.

Considering the case where the shear modulus of the particles is set to 0.01G, Fig. 10 shows the variation of predicted normal pressure on the cylindrical walls with height above base. Negative value means radially outward direction. In Fig. 10 (a), the line with the hollow triangle symbol shows the normal pressure at the end of filling, which matches well with the Janssen filling theory (the line with the solid triangle symbol) [6], with the lateral pressure ratio set to 1.0 and friction coefficient as measured at 0.24. As the vertical force was applied from the top platen, the normal pressure increased at a faster rate near the top as shown in Fig. 10 (b). Fig. 11 shows the vertical traction on the cylindrical wall against the height above base. Negative value means the downward direction. The response is similar to the normal pressure distribution towards the top but frictional traction is smaller than expected towards the bottom where friction may not be fully mobilised. Dividing this vertical traction with the normal pressure at any given point gives an indication of the "mobilised friction coefficient" at that point. The mobilized friction is smaller than the input particle-wall friction coefficient of 0.24. Fig. 12 shows the circumferential traction acting on the cylindrical walls. It can be seen that the circumferential shear is small, as we expect in an axi-symmetric system. It is interesting to note that the small circumferential traction is predicted to be positive near the top and negative near the bottom.
CONCLUSION

The chief conclusions are as follows:
Reducing particle stiffness gives a huge computational advantage, with the critical time step being inversely proportional to $\sqrt{\sigma}$. Load-displacement response depends on particle stiffness, as expected. The interpretation using Hertzian contact stiffness is being explored. The full stiffness case is currently being simulated. These results will be compared with the present results.
Reducing particle stiffness may only have secondary effects on the load transmission to the surrounding walls for a confined quasi-static system.
DEM predicted normal wall pressure distribution after filling is in good agreement with Janssen filling theory. Further analysis is underway to extend Janssen 1D analytical prediction and compare with the DEM $K_0$ compression.

ACKNOWLEDGMENTS

The authors would like to acknowledge Deere & Company, DEM Solutions Ltd. and School of Engineering & Electronics at the University of Edinburgh for funding this research. The authors are very grateful to Dipl. Ing. Johannes Härtl for his assistance in the experimental work and to Drs John Favier and Carol Plouffe for their advice and discussion about this project.

REFERENCES

Confined compression and rod penetration of a dense granular medium: discrete element modelling and validation

Y.C. Chung and J.Y. Ooi

School of Engineering & Electronics, University of Edinburgh, U.K.

Introduction

Many of the materials handled by industry each year are of a granular or particulate nature. These include pharmaceutical powders, chemical pellets, agricultural grains, coals and other minerals, sands and gravels. In recent years, the Discrete Element Method (DEM) (Cundall and Strack, 1979) has been used extensively to investigate the behaviour of granular solids subjected to a variety of loading conditions. However, the majority of the numerical computations were often not validated or compared with experimental results and there is a question as to whether DEM is capable of producing quantitative predictions rather than only qualitative representation of a particulate assembly. It is thus useful to verify DEM calculations and to investigate the relative importance of the DEM input parameters for producing satisfactory predictions.

This paper describes two physical experiments and the corresponding DEM computations of a densely packed granular medium subjected to compression and penetration. These two loading conditions were studied because they were frequently encountered in many situations where a boundary surface from an object (such as a machine or a geotechnical structure) contacts with a granular solid. The experiments consisted of an instrumented Perspex cylinder filled with granular solids. The first experiment was to compress the solid vertically under nearly $K_0$ (zero lateral deformation) condition and the second was to insert a cylindrical rod into the granular medium. The mechanical response of the granular system and the load transfer to the containing walls, the bottom platen and the penetrating rod were observed. The experiments were simulated closely using DEM and a detailed comparison between experiment and computation was made.
Both spherical (glass beads) and non-spherical (corn grains) particles were studied. Spherical particles have a tendency to rotate more than non-spherical particles and can be expected to exhibit quite different behaviour from non-spherical particles, so it is important to study both systems. The required mechanical and geometrical properties for the particles were measured carefully in laboratory tests for use in DEM computations. The sensitivity of DEM prediction to the key input parameters was also explored. The results show that DEM can produce quantitative predictions of the system studied, and that whilst it is important to use the correct particle stiffness parameter when attempting to predict the deformation response of a granular assembly, this may not be so important for producing satisfactory prediction of the force transmission in a dense quasi-static system.

Calibration experiments

The $K_0$ compression test (Fig. 1) was designed to investigate the mechanical response of a granular material under vertical loading and the load transfer to the containing walls (Masroor et al, 1987). A load was applied to a granular assembly contained in the cylinder through a top platen driven by an INSTRON machine at a constant displacement rate of 1.5mm/min. The applied load and vertical displacement were measured using the INSTRON machine. The force transmitted to the walls was measured using four strain gauges equally spaced around the cylinder walls in both circumferential and axial directions. The vertical force transmitted to the bottom platen was measured by the bottom load cell. The lateral pressure ratio $K$ and the wall friction coefficient $\mu$ can be determined using Eq. 1 where $\bar{\sigma}_v$ is the average vertical stress, $\sigma_v$ is the horizontal stress and $\bar{\tau}$ is the average shear stress, as expressed in Eq. 2.

$$K = \frac{\bar{\sigma}_v}{\sigma_v}, \quad \mu = \frac{\bar{\tau}}{\sigma_v}$$

$$\bar{\sigma}_v = \frac{2(F_r + F_B)}{\pi D^2 (1 + e_\theta)}, \quad \sigma_v = \frac{2\mu E_w (e_\theta + \nu_w e_a)}{D (1 - \nu^2)}, \quad \bar{\tau} = \frac{F_r - F_B}{\pi D h (1 - e_v)}$$

In Eq. 2: $D, t, E_w$ and $\nu_w$ are the diameter, thickness, Young’s modulus and Poisson’s ratio of the cylinder respectively; $e_\theta, e_v$ are the average hoop strain and axial strain of the cylinder at the measurement points respectively; $F_r, F_B$ are the applied load at the top platen and the measured
force at the bottom platen respectively; \( \bar{\varepsilon}_v \) is the mean vertical strain and \( h \) is the height of the granular solid.

The penetration test was designed to evaluate the resistance of granular bulk to penetration of a moving object and the dynamic force transmission to a contact surface. The experimental design is depicted in Fig. 2. The force and displacement of a rod were monitored using an INSTRON machine as the rod was pushed into granular bulk at a constant displacement rate of 50mm/min.

![Fig. 1. K\textsubscript{o} compression test setup](image1)

![Fig. 2. Rod penetration: test setup and rod dimensions](image2)

**Discrete element model**

Discrete element method is an increasingly popular numerical technique for simulating moving particles (Cundall and Strack, 1979). It is based on the use of an explicit numerical scheme in which the interactions between
a finite number of particles are monitored contact by contact and the
motion of the particles is modelled particle by particle. The particles are
rigid but deform locally at the contact points using a soft contact method.
Newton's equations of motion for each particle effectively replace the
equilibrium equations used in continuum mechanics, and the model of
inter-particle contacts replaces the constitutive model. The essential feature
of this approach is that each particle is modelled separately, so the
integrated behavior of the mass should be accurately represented, without
the need for control tests to establish constitutive models for the bulk
behavior. In this paper, a Hertz-Mindlin no-slip (Tsuji et al, 1992) contact
model with damping and a frictional slider in the tangential direction is
used, as shown schematically in Fig. 3.

Fig. 3. Non-linear spring and dashpot contact model
with a tangential slider

The DEM calculations were performed using both the EDEM code
(DEM Solutions, 2005) and the PFC3D code (Itasca, 2003). The reason
was to compare the outcomes of two independent DEM codes using
exactly the same problem configurations. The numerical samples were
prepared by filling a cylindrical container (diameter=145mm,
length=300mm) with 3591 glass beads and 4608 corn grains in each set of
computations. Both the glass beads and the corn grains did not vary
significantly in size, so particle size variation was not considered in the
numerical calculations. The corn particle was represented using
overlapping spheres (Favier et al, 1999) to match the measured average
major, intermediate and minor dimensions. A number of shape
representations are possible as shown in Fig. 4 and a 4-sphere
representation (Fig. 4c) was chosen mainly because using increasing
number of spheres to represent each particle leads to additional
computational cost. The particles were positioned in layers starting from
the base, at 1.01d centre to centre in a regular pattern with an initial
velocity of 2.56 m/s (where d=diameter of the particle). They are then
allowed to fall under gravity to achieve the initial filled state. The initial
velocity corresponds to the drop height of 335 mm used in the experiments where the particles were placed in a sieve at a height of 335 mm and allowed to "rain" through the sieve into the cylinder. This approximate particle generation scheme saves considerable computational effort, but may influence the numerical outcome since it is known that particle packing can have significant influence on bulk behaviour. The effect of this approximation was explored using different initial particle positions and will be discussed later. The particles were deemed to have settled down when the kinetic energy of the system approached zero (\(<10^{-8} \text{ J}\)) and the mean unbalanced force approached zero (\(<10^{-2} \text{ N}\)). After achieving the filled state, the \(K_0\) compression was simulated by adding a top platen and the rod penetration was simulated by adding a rod, both moving at a displacement rate of 50 mm/min.

![a) 4-sphere corn](image1.png) ![b) 6-sphere corn](image2.png)

c) geometry of 4 sphere corn particle

Fig. 4. Representations of corn grains using overlapping spheres

The boundary surfaces (the cylinder, the loading platen and the rod) were tessellated using triangular elements employing techniques common to finite element meshing (Kremmer and Favier, 2001a and b). This method allows any complex boundary surfaces to be represented relatively easily whilst maintaining computational efficiency in contact detection.
Example snapshots for the $K_0$ compression and rod penetration DEM models are shown in Fig. 5.

![Example snapshots of $K_0$ compression and rod penetration](image)

**Fig. 5.** Example snapshots of $K_0$ compression and rod penetration

### Table 1 Input parameters for glass beads

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
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<tr>
<td>Density</td>
<td>2530</td>
<td>kg/m$^3$</td>
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<tr>
<td>Diameter</td>
<td>10</td>
<td>mm</td>
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<tr>
<td>Young's modulus</td>
<td>41</td>
<td>GPa</td>
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<tr>
<td>Poisson's ratio</td>
<td>0.22</td>
<td></td>
</tr>
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<td>Friction coefficient (particle-particle, particle-wall)</td>
<td>0.24</td>
<td></td>
</tr>
<tr>
<td>Restitution Coefficient</td>
<td>0.79</td>
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</table>

### Table 2 Input parameters for corn grains

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<tbody>
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</tr>
<tr>
<td>Mass</td>
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<td>g</td>
</tr>
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<td>major dimension</td>
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<td>mm</td>
</tr>
<tr>
<td>intermediate dimension</td>
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<td>mm</td>
</tr>
<tr>
<td>minor dimension</td>
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<td>mm</td>
</tr>
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<td>Young's modulus</td>
<td>1660</td>
<td>MPa</td>
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<td>Poisson's ratio</td>
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<td>Friction coefficient (particle-particle, particle-wall)</td>
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<tr>
<td>Restitution Coefficient</td>
<td>0.59</td>
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</tr>
</tbody>
</table>

Input parameters for the glass beads and the corn grains are listed in Tables 1 and 2 respectively. The elastic modulus was determined from the single particle compression test assuming Hertzian contact. For the case of non-spherical corn, the two orthogonal curvatures at the point of contact were required and these were measured using a laser scanner. The particle-surface static friction coefficient was measured from a three-particle sliding test and the same value was adopted for the inter-particle friction. A drop test apparatus was devised to determine the resultant coefficient of
restitution. For non-spherical particle, the impact results in a more complex trajectory involving particle rotation, all of which need to be determined carefully to evaluate the restitution coefficient accurately. More details of the above characterization tests can be found in Chung et al (2004a and b).

**K₀ compression: experiment and modelling**

Figures 6a and 6b compare the load-displacement responses between DEM computation and four K₀ compression tests for glass beads and corn grains respectively. The overall trend of increasing stiffness as vertical load increases is as expected. Although each physical test followed the same filling procedure, the results show that at the initial stage when the forces are small, the loading response can vary significantly from test to test. This suggests that the natural variation in initial packing in each experiment can give significantly different loading response at low confining pressures. After this initial confinement (say after 150 N vertical force), the loading responses were largely parallel to each other, indicating that each test assembly converged to a repeatable loading response at higher confining pressures. The DEM predicted response appears to be stiffer. This is partly because the DEM model does not take into account the flexibility of the cylindrical walls (which was necessary to achieve a measurable strain to determine the loading condition). Adjusting for the additional vertical deformation deduced from the strain gauge readings was found to account for a significant part but not all of the mismatch between experiment and computation. The stiffer numerical prediction needs further investigation.

---

![Graph](image)

**a)** glass beads  
**b)** corn grains  

**Fig. 6.** Load-displacement response during K₀ compression
Figure 7 shows the force transmission onto the bottom platen during compression. Both the experimental and numerical results show the force acting on the bottom platen increases linearly with the applied vertical force. The physical tests show that only 50% of the applied load reached the bottom platen for the glass beads compared with 65% for the corn grains. Although the wall friction coefficient $\mu$ for corn is some 40% larger than for glass beads, the lateral pressure ratio $K$ for corn is significantly smaller, such that the product $\mu K$ is smaller (Eq. 1), giving a smaller share of the load acting on the cylindrical walls for the case of corn grains.

The DEM prediction is in excellent agreement with experiments for the corn grains but significantly overpredicts the force on the bottom platen for the glass beads. Further DEM calculations to explore the influence of initial filling arrangements have been conducted separately, showing that the DEM predictions are more sensitive to how the spherical glass beads are filled than non-spherical corn particles. In particular, one glass beads computation with a randomly generated initial particle positions gives a close match with the experiments, also shown in Fig. 7a. A plausible explanation is that a spherical assembly with its tendency to form crystalline structure is more sensitive to initial packing but such sensitivity is less significant for “real” particles which are predominantly non-spherical. The approximate layered initial particle positions to simulate the filling process may have contributed to this occurrence. A systematic investigation of the influence of initial packing on the loading behaviour is needed to elucidate this further.

![Force transmission onto bottom during compression](image)

a) glass beads  

b) corn grains

Fig. 7. Force transmission onto bottom during compression
Figure 8 shows the normal wall pressure distribution on the cylinder at the end of filling. This pressure distribution may be compared with the one-dimensional theory of Janssen for silo wall pressure (Janssen, 1895; Ooi and Rotter, 1990):

\[
P_n = \frac{D\gamma}{4\mu} \left(1 - e^{-z/z_0}\right) + Kq_T e^{-z/z_0}
\]

(3)

\[
z_0 = \frac{D}{4\mu K}, \quad q_T = \frac{4F_T}{\pi D^2}
\]

(4)

where \( K \) is the lateral pressure ratio, \( \mu \) is the wall friction coefficient, \( \gamma \) is the bulk density, \( z_0 \) is Janssen reference depth and \( q_T \) is the mean vertical pressure that may be applied at the top boundary (\( z=0 \)). The predicted \( K \) and \( \mu \) can be calculated from the boundary forces in the DEM results, giving \( K=0.71, \mu=0.004 \) and \( K=0.67, \mu=-0.12 \) for glass beads and corn grains respectively. The predicted mobilized friction is much smaller than the input values, which is probably a result of the dynamic filling process. The parameters \( K \) and \( \mu \) are important in the silo design and their values under vertical compression will be explored further. Using the best fit parameters from the DEM calculation, the Janssen equation matches very well with the evaluated normal pressures from contact forces.

Figure 8. Normal wall pressure distribution at the end of filling

Figure 9 shows the development of the normal wall pressures during vertical compression for both materials. The effect of vertical compression can be evaluated from the extended Janssen equation with the inclusion of an applied vertical stress at \( z=0 \) (Eq. 3). These are also plotted in Fig. 9 for comparison, using \( K \) and \( \mu \) derived from DEM results. Since Janssen is a one-dimensional theory that does not take into account the top and bottom
boundary conditions, there is significant mismatch especially towards the boundaries.

Dividing the vertical traction with the normal pressure at any given point on the wall gives an indication of the "mobilised friction coefficient" at that point. Figure 10a shows that the mobilised wall friction at the five calculation positions are within the range of 0.07-0.17 for the glass beads, significantly smaller than the input particle-wall friction coefficient of 0.24. This is in agreement with previous studies (Rotter et al, 1998) showing significantly smaller macroscopic friction than the inter-particle microscopic friction for a spherical assembly. For the corn grains, a higher mobilized friction coefficient is achieved with values of 0.21–0.31 when the vertical force is close to 1000 N (this compares with input friction coefficient of 0.34). The tendency for perfect spheres to rotate more as compared to non-spherical particles may be one main reason for the much smaller macroscopic friction. Circumferential traction acting on the cylinder was also evaluated and found to be relatively small, as expected in an axisymmetric system.

![Fig. 9. Normal wall pressure distribution during compression](image-url)
The lateral pressure ratio $K$ was evaluated from the experimental data using Eq. 1 and plotted against the DEM prediction in Fig. 11. The experimental results are reasonably repeatable for each material, showing a trend of the $K$ value increasing and reaching a stable value of $\sim 0.4$ for glass beads and $\sim 0.35$ for corn grains, with a larger scatter for the glass beads. The DEM prediction for the corn computation is in excellent agreement but for the sphere assembly, DEM predicts a much larger $K$ value of $\sim 0.62$. 

(a) glass beads
Rod penetration: experiment and modelling

The load-displacement responses for the rod penetration into glass beads and corn grains are shown in Fig. 12. These computations were performed with particle shear modulus $G$ decreased to $0.01G$ to reduce computational effort. In addition, for the glass beads computation, a further computational advantage was gained by increasing the density $\rho$ to $1000\rho$. Density scaling has been used successfully in previous studies (e.g. Zhang, 2003). The measured force fluctuated significantly during penetration into each material, but the average trend is repeatable with the corn grains giving a larger resistance to penetration. The DEM results also fluctuated in a seemingly similar fashion and show a good quantitative match with the experiments in each material.
Influence of input parameters

The calculations above were all performed using material parameters as measured from laboratory tests. Further calculations were conducted to explore the sensitivity of the input parameters on the numerical outcomes. One other objective was to investigate the methodology for reducing DEM computational time since the calculation time step is inversely proportional to $\sqrt{G/\rho}$, where $G$ is the shear modulus and $\rho$ is the density of particles. Due to space constraint, only part of the results will be presented here.
DEM computations were conducted with particle shear modulus reduced to $10^{-2}G$, $10^{-3}G$ and $10^{-4}G$. For the load-displacement response in $K_o$ compression which is strongly dependent on the bulk stiffness of the assembly, reduced particle stiffness results in a softer response as expected. Figure 13 shows the force acting on the bottom platen during vertical compression for the cases of full stiffness and 100 times smaller stiffness. The results show that when particle stiffness is reduced by 100 times, the proportion of the applied force transmitted to the bottom platen reduced by ~10% for glass beads and there is no noticeable difference in the results for corn grains. The results show that for this confined quasi-static system, reducing the particle stiffness by a few orders may have only secondary effects on the load transfer mechanism.

![Graphs showing force vs. top force for glass beads and corn grains](image)

a) glass beads  
b) corn grains

Fig. 13. Effect of shear modulus on predicted response for $K_o$ compression

**Conclusions**

Discrete element modelling of $K_o$ compression and rod penetration into a spherical and a non-spherical granular assemblies have been presented. The physical experiments were performed with care which include direct laboratory measurements of the key DEM input parameters. Comparisons have been made between the numerical results and the experiments.

The study has shown that for the corn grains, the DEM predictions are in good agreement with the experiments for all cases studied. This provides some verification that DEM is capable of producing quantitative predictions. The results also suggest that very accurate representation of the particle shape may not be necessary to produce satisfactory predictions and capturing the key linear dimensions of a particle may be adequate.
The DEM results for the spherical glass beads were not always in good agreement with the experiments. DEM predictions have been found to be more sensitive to how the spherical glass beads are filled than nonspherical corn particles. The spherical assembly appears to be more sensitive to initial packing structure resulting from how the particles are generated initially. The sensitivity of DEM computations to initial packing structure needs further study.

The sensitivity of DEM prediction to the stiffness parameter was also explored. It has been found that reducing the particle stiffness by a few orders only has secondary effects on the load transmission in the quasi-static assembly. Since contact forces propagate through the granular assembly to transmit to the boundary surfaces, the development of the force chains and the internal states of stress and strain within the assembly is important and is currently under investigation.

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Measurement and modelling of a particulate assembly under confined compression

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ABSTRACT

The Discrete Element (DE) method has been used extensively in recent times to study the behaviour of particulate assemblies. However, the numerical simulations are often not validated or compared with the experimental results. This paper describes the experiment and DE simulation of a confined compression test to investigate the mechanical response of a dense particulate system and the load transfer to the containing walls under vertical compression. After the particles were filled in the cylinder, a load was applied to the particulate assembly contained in the cylinder through a top platen driven by an INSTRON machine. The vertical load and vertical displacement was measured during loading. The forces transmitted to the walls were measured by using strain gauges fixed to the cylinder wall in both circumferential and axial directions. In addition, the vertical force transmitted to the bottom of the cylinder was also measured with another load cell on the bottom platen. The required mechanical and geometrical properties of the particles for use in the DE simulations were measured carefully in laboratory tests. A systematic investigation of the influence of initial packing on the loading behaviour was carried out. Comparisons between the numerical results and the experimental results were presented and discussed.

Keywords: DEM; Particulate material; Confined compression; Particle packing

1 INTRODUCTION

Many of the materials handled by industry each year are of a granular or particulate nature. These include pharmaceutical powders, chemical pellets, agricultural grains, coals and other minerals, sands and gravels. Particles undergo a variety of stress and deformation regimes during many industrial processes. In order to model such processes, the Discrete Element Method (DEM) (Cundall and Strack 1979) has been used extensively to investigate the behaviour of granular solids. However, the majority of the numerical computations were often not validated or compared with experimental results and there is a question as to whether DEM is capable of producing quantitative predictions rather than only qualitative representation of a particulate assembly. This paper describes a confined compression experiment to validate the corresponding DEM simulations, and to investigate the mechanical response of a particulate assembly under confined compression. The experiment consisted of an instrumented Perspex cylinder filled with particles. After the particles have settled down, a top platen was applied to compress the bulk solid vertically. The load transfer to the containing walls and the bottom platen was observed. The experiment was simulated closely using DEM and the required mechanical and geometrical properties for the particles were measured carefully in laboratory tests for use in DEM computations. The effect of particle packing was explored in this study. A detailed comparison between experiment and computation was made.

2 CONFINED COMPRESSION EXPERIMENTAL SETUP

The confined compression test, as shown in Fig. 1, was designed to investigate the mechanical response of a granular material under vertical loading and the load transfer to the containing walls (Masroor et al 1987). A load was applied to a granular assembly contained in the cylinder through a top platen driven by an INSTRON machine at a constant displacement rate of 1.5 mm/min. The applied load and vertical displacement were measured using the INSTRON machine. The force transmitted to the walls was measured using four strain gauges equally spaced around the cylinder.
wall in both circumferential and axial directions. The vertical force transmitted to the bottom platen was measured by the bottom load cell. This physical experiment thus provides a good method for observing the behaviour of a dense particulate system under confined compression and the transfer of force through friction onto the boundary surfaces.

![Diagram of test setup](image)

**Fig. 1. Confined compression test setup**

### 3 NUMERICAL PROCEDURE AND INPUT PARAMETERS

Discrete element method is an increasingly popular numerical technique for simulating moving particles. It is based on the use of an explicit numerical scheme in which the interactions between a finite number of particles are monitored contact by contact and the motion of the particles is modelled particle by particle. The particles are rigid but deform locally at the contact points using a soft contact method. Newton’s equations of motion for each particle effectively replace the equilibrium equations used in continuum mechanics, and the model of inter-particle contacts replaces the constitutive model. The essential feature of this approach is that each particle is modelled separately, so the integrated behavior of the mass should be accurately represented, without the need for control tests to establish constitutive models for the bulk behavior. In this paper, a Hertz-Mindlin no-slip (Tsuji et al. 1992) contact model with damping and a frictional slider in the tangential direction is used.

The DEM calculations were performed using both the EDEM code (DEM Solutions 2005) and the PFC3D code (Itasca 2003). The reason was to compare the outcomes of two independent DEM codes using exactly the same problem configurations. Since particle packing may have significant influence on bulk behaviour, the effect of particle packing was explored using different initial particle positions. The numerical samples were prepared by filling a cylindrical container (diameter=145mm, length=300mm) with 3591 glass beads. The glass beads did not vary significantly in size (diameter=10mm, tolerance=+/-0.5mm), so particle size variation was not considered in the numerical calculations. The glass beads were positioned in layers starting from the base, at 1.01d, 1.50d, and 2.00d (where d= diameter of the glass bead) centre to centre in a regular pattern with an initial velocity of 2.56 m/s. They are then allowed to fall under gravity to achieve the initial filled state. The initial velocity corresponds to the drop height of 335 mm used in the experiments where the particles were placed in a sieve (grid separation = 15 mm) at a height of 335 mm and allowed to "rain" through the sieve into the cylinder. In addition to the above approximate particle generation scheme, the glass beads were positioned according to the face-centred cubic (FCC) array, rhombic array and random generation starting from the base with a zero initial velocity and then allowed to settle under gravity. The particles were deemed to have settled down when the kinetic energy of the system approached zero (<10^-8 J) and the mean unbalanced force approached zero (<10^-5 N). After achieving the filled state, the confined compression was simulated by adding a top platen, moving at a displacement rate of 50 mm/min.

Input parameters for the glass beads are as follows: the density is 2530 kg/m³; the Young’s modulus is 41 GPa; the Poisson’s ratio is 0.22; the friction coefficient is 0.24; the coefficient of restitution is 0.79. The elastic modulus was determined from the single particle compression test assuming Hertzian contact. The particle-surface static friction coefficient was measured from a three-particle sliding test and the same value was adopted for the inter-particle friction. A drop test apparatus was devised to determine the resultant coefficient of restitution. More details of the above characterization tests can be found in Chung et al. (2004a and b).
4 COMPARISON BETWEEN EXPERIMENT AND SIMULATION

The influence of the initial particle arrangements was explored by comparing the force transmission onto the bottom platen in the DEM computations with the experiments. Figure 2a shows the DEM predictions for the three particle generation schemes with particle separations 1.01d, 1.50d and 2.00d. Figure 2b shows the DEM results for particles generated according to FCC array, rhombic array and random generation. The case with particles packed randomly and the cases with initial particle separations of 1.50d and 2.00d all have very good agreement with the experiments, with the exception that a local failure occurred in the random generation case. This suggests that particle separation larger than 1.50d is sufficient to produce the packing arrangement achieved in the filled state. It is not surprising that the denser rhombic and FCC packing predicted much larger forces being transmitted onto the bottom platen. The case with particle separation of 1.01d also predicted a larger force, indicating that the small separation was not sufficient to allow the particles to settle to the packing structure achieved in the experiments. These computations highlight the importance of correct representation of the initial packing structure in DEM calculations. If the initial packing is modelled correctly, the present DEM predictions match very well with the experimental results, showing that the force acting on the bottom platen increases linearly with the applied vertical force, with ~50% of the applied load reaching the bottom platen.

![Figure 2a: Force transmission onto the bottom platen: 1.01d, 1.50d and 2.00d](image1)

![Figure 2b: Force transmission onto the bottom platen: FCC, rhombic and random packing](image2)

Focusing on the DEM prediction with particle separation of 1.50d (equal to the sieve grid separation of 15 mm), Fig. 3a compares the displacement-load response between the DEM prediction and three confined compression tests. The overall trend of increasing stiffness as vertical load increases is as expected. Although each physical test followed the same filling procedure, the results show that at the initial stage when the forces are small, the loading response can vary significantly from test to test. The natural variation in initial packing in each experiment can give significantly different loading response at very low confining pressures. After this initial confinement (say after 150 N vertical force), the loading responses were largely parallel to each other, indicating that each test assembly converged to a repeatable loading response at higher confining pressures. Focusing on the response after initial confinement, the DEM predicted a stiffer response. This is partly because the DEM model did not take into account the flexibility of the cylindrical walls, which was necessary to achieve a measurable strain to determine the loading condition. Adjusting for the additional vertical deformation deduced from the strain gauge readings was found to account for a significant part but not all of the mismatch between experiment and computation. The stiffer numerical prediction needs further investigation.

Figure 3b shows the normal wall pressure distribution on the cylinder at the end of filling and during compression. At the end of filling the normal wall pressure near the top is smaller than that near the bottom due to gravity, and it becomes progressively larger during compression. This pressure distribution may be compared with the one-dimensional theory of Janssen for silo wall pressure (Janssen 1895; Ooi and Rotter 1990):
where $K$ is the lateral pressure ratio, $\mu$ is the wall friction coefficient, $\gamma$ is the bulk density, $D$ is the diameter of the cylinder, $z$ is the depth from the top surface, and $F_T$ is the applied vertical load at the top boundary ($z=0$). The $K$ and $\mu$ can be calculated from the boundary forces in the DEM results. At the end of filling ($F_T=0$), we obtain $K=0.9$, $\mu=0$. The zero friction is probably influenced by the DEM simulation of the dynamic filling process and the scale of the problem studied. Using the best fit parameters from the DEM calculation, the Janssen pressures at the end of filling match very well with the evaluated normal pressures from the contact forces. The effect of vertical compression can be evaluated from the extended Janssen equation with the inclusion of an applied load $F_T$ (Eq. 1). These are also plotted in Fig. 3b for comparison, using $K$ and $\mu$ derived from the DEM results. Since Janssen is a one-dimensional theory that does not take into account the top and bottom boundary conditions, there is significant mismatch especially towards the boundaries. Dividing the vertical traction with the normal pressure at any given point on the wall gives an indication of the "mobilised friction coefficient" at that point. When the vertical force is close to 932 N, the mobilised wall friction coefficient at the six calculation positions are within the range of 0.14-0.16, significantly smaller than the input particle-wall friction coefficient of 0.24. This is in agreement with previous studies (Rotter et al 1998) showing significantly smaller macroscopic friction than the inter-particle microscopic friction for a spherical assembly.

The parameters $K$ and $\mu$ are important in the silo design, so their values under vertical compression should be explored further. The two parameters can be determined from the experiments using Eq. 2.

$$K = \frac{\sigma_H}{\sigma_v}, \quad \mu = \frac{\tau}{\sigma_H} \quad (2)$$

where $\sigma_v$ is the average vertical stress, $\sigma_H$ is the horizontal stress at the measurement point and $\tau$ is the average shear stress, as expressed in Eq. 3.

$$\sigma_v = \frac{2(F_T + F_B)}{\pi D (1 + \epsilon_\theta)^2}, \quad \sigma_H = \frac{2t E_w (\epsilon_\theta + \nu \epsilon_a)}{D (1 - \nu)^2}, \quad \tau = \frac{F_T - F_B}{\pi Dh (1 - \epsilon_v)} \quad (3)$$

In Eq. 3: $E_w$, $\nu_w$ and $t$ are the Young's modulus, Poisson's ratio and thickness of the cylinder respectively; $\epsilon_\theta$, $\epsilon_a$ are the average hoop strain and axial strain of the cylinder at the measurement points respectively; $F_T$, $F_B$ are the applied load at the top platen and the measured force at the bottom platen respectively; $\epsilon_v$ is the mean vertical strain and $h$ is the height of the granular solid. Figures 4a and 4b compare the parameters $K$ and $\mu$ between DEM prediction at different heights above the base (i.e. 10, 50, 90, 130 and 170mm) and three confined compression tests. The experiments were reasonably repeatable, showing a trend of the $K$ and $\mu$ values reaching a stable value of ~0.45 and ~0.25 respectively. The DEM predicts larger $K$ value and lower $\mu$ value.
Discrete element modelling of confined compression of a spherical granular assembly has been presented. The results were compared with the equivalent physical experiments, including direct laboratory measurements of the key DEM input parameters. A systematic investigation of the influence of initial packing on the loading behaviour was carried out, which demonstrated the influence of initial packing structure on the bulk behaviour. The DEM results for the spherical glass beads were not always in good agreement with the experiments. Further DEM validation study using non-spherical particles (corn grains) have been conducted which showed considerably better agreement with the experiments (Chung and Ooi 2005). Spherical assemblies appear to be more sensitive to initial packing structure resulting from how the particles are generated initially. One explanation is that DEM model of perfect spheres, which have a tendency to form crystalline structure and a tendency to rotate more than non-spherical particles, is not an appropriate representation of the glass beads with their natural imperfections.

Fig. 4. Comparison of a) predicted lateral pressure ratio and b) predicted wall friction coefficient with experiment

6 REFERENCES


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