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An investigation of fabric and of particle shape in railway ballast using X-ray CT and the discrete element method

A thesis submitted in fulfilment of the requirements for the degree of
Doctor of Philosophy

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UNIVERSITY OF SOUTHAMPTON  

**Abstract**  

FACULTY OF ENGINEERING AND THE ENVIRONMENT  
SCHOOL OF CIVIL ENGINEERING  
Doctor of Philosophy  

**AN INVESTIGATION OF FABRIC AND OF PARTICLE SHAPE IN RAILWAY BALLAST USING X-RAY CT AND THE DISCRETE ELEMENT METHOD**  

Sharif Iftekhar Ahmed  

The mechanical behaviour of uncedmented granular matter is influenced by the grain shape (i.e. form, angularity and concavity) and the material’s fabric (i.e. the spatial arrangement of particles and contacts). Discrete element modelling has been used in the past to compare different shaped particles (e.g. spheres, ellipsoids, etc.) but without any clear quantitative link to the shape of real materials. Existing methods of direct observation of fabric are restricted to sands (i.e. in the sub-millimetre particle scale) that bear little relation to gravel sized material and above, such as railway ballast, which is typically an order-of-magnitude larger and much different in shape.  

*Non-destructive, micro-focus X-ray Computed Tomography (XCT) imaging in 3D is used to visualise, quantify and assess the fabric of intact large-scale ballast bed sections and complete 150 mm diameter laboratory element test specimens for the first time. Shape information obtained by detailed 3D characterisation of real ballast particles has been used to create a library of representative ‘DEM ballast particles’ that are employed (in a new triaxial shear model based upon the principles of potential particles) to investigate, isolate and elucidate the impact of particle shape on mechanical and fabric response observed in railway ballast.*  

Fabric in railway ballast experiences load induced changes (primarily) through the breaking and/or forming of (new) contacts points and increased anisotropic intensity of contact orientations in favour of the load path. This is accompanied by some loss in anisotropy of the particles orientation but this is not significant
indicating that confinement of surrounding particles (in the crib and shoulder) inhibit particle movements. A 90° stress rotation appears to alter the fabric in such a way that reverting to the original loading path does not recover the original fabric. This is true for particle and contact orientation fabric. In the volumetric response domain, form (i.e. the 3D proportions of the particle) changes the packing characteristics such that greater compression is seen during initial stages of shear. While angularity and concavity increase the rate of dilation, the latter has the greatest rate change. With greater shape complexity (form→angularity→concavity), stronger mobilised strength characteristics are also seen. In the domain of fabric, particle rotation is the principal parameter controlling how the structure in granular materials behaves under loading. As the shapes tends towards realistic concave objects, stronger more resilient fabric develops that impedes rotation through a combination of improved packing, higher contact coordination number and increased intensity of contact orientation anisotropy.
To my Mom,

having sacrificed much to raise her own to great heights.

And to my Dad,

who will have been proud.
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Nomenclature

\( \theta \)  
Angles

\( \psi \)  
Zenith (inclination) angles

\( \phi \)  
Azimuth angles

\( \lambda \)  
Scalar

\( \lambda \)  
X-ray wavelengths

\( \Lambda \)  
Lagrangian multiplier

\( \rho \)  
Particle Density

\( \phi_p \)  
Inter-particle friction angle

\( \beta_i \)  
Shape factor

\( \beta_i \)  
Strength factor

\( \sigma_a \)  
A Proportionality constant

\( \varepsilon_a \)  
Global axial strain

\( \varepsilon_a \)  
Axial strain

\( \psi_c \)  
Inclination angle

\( \psi_c \)  
Contact normal orientation

\( \phi^\prime_{\text{crit}} \)  
Critical state strength

\( \alpha_d \)  
Damping Constant

\( \psi_{\text{maj}} \)  
Zenith angles for the major axis

\( \theta_{\text{maj}} \)  
Azimuth angles for the major axis

\( \psi_{\text{min}} \)  
Zenith angles for the minor axis

\( \theta_{\text{min}} \)  
Azimuth angles for the minor axis

\( \phi^\prime_{\text{mobs}} \)  
Mobilised shear strength

\( \phi^\prime_{\text{peak}} \)  
Peak strength

\( \varepsilon_q \)  
Shearing strain rate

\( \alpha_o \)  
Timestep Safety Factor

\( \alpha_o \)  
Safety factor

\( \varepsilon_v \)  
Volumetric strain

\( \vartheta \)  
Column vector

2D  
Two dimension / two dimensional

3D  
Three dimension / three dimensional

\( A \)  
Area of the object

\( A_p \)  
Area of a circle with the same perimeter as the object

ARU  
Arundel

ASF  
Aggregate shape factor

\( C \)  
Speed of light
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>Compton scatter</td>
</tr>
<tr>
<td>CAM</td>
<td>Camberley</td>
</tr>
<tr>
<td>CCD</td>
<td>Charge-coupled Device</td>
</tr>
<tr>
<td>CH</td>
<td>Cliffe Hill</td>
</tr>
<tr>
<td>CLDA</td>
<td>Curved Linear Detector Array</td>
</tr>
<tr>
<td>CN</td>
<td>Contact coordination number</td>
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<tr>
<td>CPS</td>
<td>Concave Particle Specimen</td>
</tr>
<tr>
<td>CR</td>
<td>Concavity Ratio</td>
</tr>
<tr>
<td>CT</td>
<td>Computed tomography</td>
</tr>
<tr>
<td>DB</td>
<td>DEM ballast</td>
</tr>
<tr>
<td>DBS</td>
<td>BEM Ballast Specimen</td>
</tr>
<tr>
<td>DEM</td>
<td>Discrete element method</td>
</tr>
<tr>
<td>$D_{eq}$</td>
<td>Equivalent disc diameter</td>
</tr>
<tr>
<td>$D_{max}$</td>
<td>Maximum diameter</td>
</tr>
<tr>
<td>$D_{min}$</td>
<td>Minimum diameter</td>
</tr>
<tr>
<td>$d_{x}$</td>
<td>Incremental thickness of material traversed</td>
</tr>
<tr>
<td>$e$</td>
<td>Void ratio</td>
</tr>
<tr>
<td>$E$</td>
<td>Ellipseness</td>
</tr>
<tr>
<td>$E_{c}$</td>
<td>Elastic constant modulus</td>
</tr>
<tr>
<td>$E_{e}$</td>
<td>Elastic contact modulus</td>
</tr>
<tr>
<td>$e_{ct}$</td>
<td>Void ratio measurements from the CT data</td>
</tr>
<tr>
<td>EIE</td>
<td>Equivalent inertia ellipse diameter</td>
</tr>
<tr>
<td>$e_{lab}$</td>
<td>Void ratio measurements from the laboratory</td>
</tr>
<tr>
<td>EPS</td>
<td>Ellipsoidal Particle Specimen</td>
</tr>
<tr>
<td>eV</td>
<td>Electron volts</td>
</tr>
<tr>
<td>$E_{x}$</td>
<td>Energy</td>
</tr>
<tr>
<td>$e_{x}$</td>
<td>Vertical standard basis</td>
</tr>
<tr>
<td>F</td>
<td>Fabric tensor</td>
</tr>
<tr>
<td>G</td>
<td>Particle material shear modulus</td>
</tr>
<tr>
<td>GBE</td>
<td>Geometric Best-fit Ellipse</td>
</tr>
<tr>
<td>GS</td>
<td>Glensanda</td>
</tr>
<tr>
<td>H</td>
<td>Homoplaty</td>
</tr>
<tr>
<td>$H$</td>
<td>Planck’s constant ($6.63 \times 10^{-34}$ Js)</td>
</tr>
<tr>
<td>HMA</td>
<td>High Marnham</td>
</tr>
<tr>
<td>I</td>
<td>Intermediate orthogonal axis</td>
</tr>
<tr>
<td>$I$</td>
<td>Intensity</td>
</tr>
<tr>
<td>$I_{1}$</td>
<td>Intermediate dimension perpendicular to $L$</td>
</tr>
<tr>
<td>$1/L$</td>
<td>Elongation</td>
</tr>
<tr>
<td>ICC</td>
<td>Inscribed and circumscribed circle diameter</td>
</tr>
<tr>
<td>$I_{n}$</td>
<td>Inertia number</td>
</tr>
<tr>
<td>IQR</td>
<td>Inter-quartile range</td>
</tr>
</tbody>
</table>
IS  
Intercept sphericity

$K$  
Inter-particle contact stiffness

$k^{rot}$  
Rotational motion

$k^{tran}$  
Translational motion

$L$  
Longest orthogonal axis

$L$  
Longest dimension of the particle

LASS  
Laser-based Aggregate Scanning

LRig  
SRTF sample

LS  
Least Squares method

$mCN$  
Mechanical (contact) coordination number

MPS  
Maximum Projection Sphericity

MRI  
Magnetic Resonance Imaging

$n$  
Porosity

$N$  
Number of squares

$N_i$  
Number of particles with one contact

$N_c$  
Total number of contacts

$n_{k}$  
Unit orientation vector of the $k$th particle

$N_o$  
Number of particles with zero contact

$N_p$  
Number of particles

NR  
Network Rail

$NRF$  
Nuclear roundness factor

NWM  
New Milton

$n_i$  
Number of atoms/cm$^3$

$P$  
Perimeter of the object

PE  
Photoelectric effect

$PR$  
Percentage roundness

PSD  
Particle Size distribution

PSD  
Particle Size Distribution

PVE  
Partial volume effect

$r_a$  
Radius of a circle with the same area

RGB  
Red, green and Blue colour coordinates

$r_p$  
Radius of a circle with the same perimeter as the object

RRV  
Rail Road Vehicle

$S$  
Smallest orthogonal axis

$S$  
Smallest dimension perpendicular to both $L$ and $I$

$S/I$  
Flatness

$S/L$  
Equancy

$S^2$  
Sample homogeneity index

$S^2$  
Sample homogeneity index

$SF$  
Surface factor

$S_{sh}$  
Shear waves, horizontally propagating horizontally polarised

xxii
$S_{sv}$ Shear waves, horizontally propagating vertically polarised
SPS Spherical Particle Specimen
SRTF Southampton Railway Testing Facility
SSPS Single Shape Particle Specimen
ssTEM Serial-section transmission electron-microscopy
$S_{sh}$ Shear waves, vertically propagating horizontally polarised
T1 Cyclic compression
T2 Cyclic compression and extension
T3 Cyclic compression – extension – compression
$t_{crit}$ Critical timestep
TiO$_2$ Titanium dioxide
TSA Trainable segmentation algorithm
UIAIA University of Illinois Aggregate Image Analyser
UID Unique Identification
$U_n$ Unit normal vector
$v$ Specific volume
$V^i$ Velocity of the particle
$V_n$ Normal vector
$V_s$ Volume of solid particles
$V_v$ Volume of voids
$X$ Local coordinate vector
XCT X-ray Computed Tomography
$\sigma_1$ Major principal stress
$\sigma'_1$ Effective major principal stress
$\sigma_2$ Intermediate principal stress
$\sigma'_2$ Effective intermediate principal stress
$\sigma_3$ Minor principal stress
$\sigma'_3$ Effective minor principal stress
Declaration Of Authorship

I, Sharif I. Ahmed, declare that the thesis entitled *An investigation of fabric and of the effects of particle shape in railway ballast* and the work presented in it are my own. I confirm that:

- this work was done wholly while in candidature for a research degree at this University;
- where any part of this thesis has previously been submitted for a degree or any other qualification at this University or any other institution, this has been clearly stated;
- where I have consulted the published work of others, this is always clearly attributed;
- where I have quoted from the work of others, the source is always given. With the exception of such quotations, this thesis is entirely my own work;
- I have acknowledged all main sources of help;
- where the thesis is based on work done by myself jointly with others, I have made clear exactly what was done by others and what I have contributed myself;

- parts of this work have been published as


Signed: ___________________________ Date: ___________________________
1

Introduction

1.1. Background

Traditional railway tracks consist of four basic components: running rails, sleepers, ballast, and the sub-base (Figure 1.1). Load applied by the passage of trains is transmitted through the rail-sleeper system onto the ballast layer where the stresses are spread to levels acceptable for the underlying sub-base. It is now generally accepted that good-quality hard angular stones (e.g. granite) (Claisse & Calla, 2006), free from dust and dirt, are the best material for ballast. This has obvious advantages as it allows for rapid drainage, optimum stiffness and an ability to be mechanically tamped for improvement to track evenness when necessary.

![Figure 1.1 Schematic cross section through a railway track](image)

By weight and by volume, ballast aggregates is the largest component of the conventional rail track, and the cost of buying and distributing ballast forms a significant part of the entire civil engineering budget of the railway operators around the world (Cope, 1993). In spite of the fact that ballast is the most important component of the permanent way, most attention has been focused on
the track superstructure of rails, fasteners and sleepers, and until recently not much consideration has been given to understanding the behaviour of ballast in detail (Selig & Waters 1994).

Conventional track design generally ignores the granular nature of the ballast particles that make up the ballasted bed (Burrow et al., 2007). This is because of a lack of understanding of complex particle breakage mechanisms and the absence of a realistic stress-strain constitutive model which includes plastic deformation, particle breakage and particle rearrangement under a large number of load cycles (Salim 2004). As a result, track designs tend to be empirical and have technical shortcomings in their construction such as the use of a universal ballast particle gradation irrespective of local ground/environmental conditions (Burrow et al., 2007). This can lead to shorter periods of serviceability because of defects such as differential settlement of the track bed and misalignment of the rails. Remedial measures such as tamping can be used to temporarily correct the track geometry in the short term. This is done by lifting the sleeper and inserting a set of vibrating arms or tines into the ballast crib/shoulder on either sides of the sleeper which are then moved towards each other to push the ballast under the sleeper. This technique tends to damage the ballast particles and generates fines. More importantly, tamping destroys the arrangement and orientation (structure) of the ballast particles that has occurred due to traffic loading over a period of time. As a direct result, there is a temporary loss of stiffness of the track and measures such as speed restrictions and dynamic track stabilisation must be applied in order to restore the structure in the ballast that was present prior to maintenance.

The structure that develops as a result of traffic/cyclic loading can be adequately described as fabric or in other words the interlocking between angular particles. Researchers have shown that fabric in a granular material such as ballast (lacking any form of cementation) plays a very important role in its mechanical behaviour and resilient responses to loading (Cresswell and Barton, 2003).

Given its importance, there is very little scientific understanding of fabric structure in a ballasted track and its development through the various stages of the ballast/track life cycle i.e. from construction to renewal. A detailed
understanding will enable the operators to minimise the need for aggressive maintenance procedures (such as tamping) and develop advanced track design and less damaging maintenance regimes that are not only cost effective but also provide improved service life.

Furthermore, a clear understanding of the shape characteristics of ballast would allow for a greater appreciation of the effects of loading on the individual particles’ life cycle. This knowledge is also vital to study the effects of fabric structure, since it is hypothesised that interlocking is wholly dependent on the characteristics of the particles involved.

1.2. Aims and objective of research

The primary goal of this research is to investigate the influence of the different particle shape parameters (e.g. form, angularity) on the strength, deformation and fabric (interlocking) characteristics of railway ballast under loading.

The key objectives of the project are to,

1. Develop a robust and cost effective method of 3D particle characterisation using image based technologies and subsequently characterise the shape of industry standard railway ballast.
2. Create a library of numerical DEM particles that have similar shape as the real ballast that has been characterised.
3. Develop, calibrate and test a DEM triaxial cell model to be used for the study of particle shape parameters.
4. Develop a means of analysing and quantifying the fabric of the ballast bed of a railway track (undisturbed) for comparison with numerical results.

1.3. Methodology

The research objectives were divided in to two workflow paths. The first three objectives are sequentially linked and makeup Workflow – 1. Objective four formed a parallel workflow since it was not dependent on any output from Workflow-1. Figure 1.2 illustrates the key steps taken to fulfil the aims and objectives of this work.
1.3.1. Workflow - 1
This part of the work started off by securing a quantity of Network Rail specification ballast. The ballast was washed and a PSD analysis was carried out. Particles were then chosen at random and photographed from three orthogonal views. A series of algorithms were implemented in MATLAB to carry out automated feature extraction, dimension analysis and shape characterisation on the captured images. The shape information of the real ballast was then used to construct realistic DEM ballast particles that are of similar shape characteristics to the physical ballast. A new numerical triaxial cell test model was tested parametrically using the DEM ballast and later calibrated to laboratory triaxial experiments carried out on 1/3 scale ballast having the same shape characterises and originating from the same source as the imaged ballast. The calibrated model was then used to simulate monotonic triaxial shear tests to investigate the mechanical significance of the different shape parameters with respect to railway ballast.

1.3.2. Workflow – 2
A method of retrieving preserved specimens from the ballast bed was developed for application under field conditions. High energy X-ray Computed Tomography (XCT) was used to image the internal structure of field and complete laboratory triaxial tests specimens in three dimensions (3D). The data were then used to investigate the fabric that develops under field/laboratory conditions and the effects of load reversal on the internal structure of gravel sized granular matter.

1.4. Outline of the thesis
This thesis is organised into seven chapters.

This chapter, Chapter 1, gives an introduction to the thesis topic as well as a description of the main aim and associated objectives of the research, the overall methodology and the thesis outline

Chapter 2 presents an overview of the current understanding of the fabric in granular soils. The effect of fabric on the strength and stiffness of natural sand formations and laboratory soil specimens are discussed. The approaches available
to obtain data to quantify fabric and the parameters used are presented. Micro-
scale observations of the effects on the mechanical response of the material and
the evolution of fabric under loading are also described. As fabric and particle
morphology are related the last part of this chapter considers previous studies of
the effects of particle size and shape of coarse grained materials. Experimental
and numerical evidence of the importance of size and shape on the mechanical
behaviour of granular systems is summarised and previous methodologies used to
measure particle size and shape are discussed.

Chapter 3 describes the development and application of a field-scale ballast bed
sampling method that preserves the fabric. A brief background into the theory
and implementation of industrial XCT equipment is put forward followed by a
description of the 3D imaging and image processing protocols developed to allow
the analysis of fabric of intact gravel sized granular systems.

Chapter 4 presents the current state-of-the-art for image based measurement
techniques associated with particle shape. It then describes the development of a
3D particle imaging capture system the output of which is used to implement a
new technique for shape characterisation of real ballast. Finally, a library of
virtual numerical ballast particles is created based on these measurements.

Chapter 5 starts by introducing the theory of the Discrete Element Method
(DEM) and the underling concepts behind potential particles. The method used
to create DEM triaxial specimens is described and followed by a detailed
parametric study to analyse impact of different numerical and mechanical
variables on simulations. Finally, the DEM modelling parameters are calibrated
against laboratory triaxial test results.

In Chapter 6 the effects of particle shape parameters (e.g. form and angularity)
on the mechanical and fabric response of railway ballast is investigated

Finally, Chapter 7 presents a summary of the work undertaken in this study,
the key conclusions and recommendations for future research.
Figure 1.2 Overall methodology flowchart
2

Literature review

2.1. Introduction

Granular media such as ballast consist of discrete particles in contact with each other that form a connected matrix giving it its strength. When stressed, the matrix changes by reordering the particle configuration (translating and or rotating) as the applied load passes through the material. Evidence of this rearrangement of particles can, for example, be observed in the form of volume change upon shearing or liquefaction of sands under cyclic loading. In spite of this, geotechnical analysis of granular soils is carried out primarily on the basis of continuum theories such as the elasticity and plasticity theories. These are phenomenological approaches that replace the real material by a mathematical model of a structure-less homogenous mass and it is assumed that the material experiences isotropic stress and strain when loaded.

Terzaghi (1920), in a discussion of the assumptions on which traditional continuum theories are based, wrote:

“The fundamental error was introduced by Coulomb, who purposely ignored the fact that sand consists of individual grains, and who dealt with the sand as if it were a homogeneous mass with certain mechanical properties. ...... but it developed into an obstacle against further progress as soon as its hypothetical character came to be forgotten by Coulomb’s successors. The way out of the difficulty lies in dropping the old fundamental principles and starting again from the elementary fact that sand consists of individual grains”

Incomplete understanding of the physical particle-scale mechanisms governing soil deformations and the paucity of reliable data for quantifying the arrangements of
particles has inhibited a more complete description of the behaviour of these materials.

To understand how fabric (i.e. the inter-particle locking) influences the macro-scale response and predict fabric evolution, an understanding of the physical mechanisms mobilized in response to the applied external stresses is required. Given the difficulty of analysing internal deformation of real granular media at the particle scale, current understanding of the link between particle interactions and the macro-scale response comes either from discrete element modelling (DEM) or two-dimensional physical models, often using photoelastic materials.

This chapter presents a brief overview on current knowledge of fabric associated with granular media. The effect of fabric on the strength and stiffness is explored and examples given of directional dependence or anisotropy of the constituent particles within granular media.

2.2. Defining fabric

The concept of ‘fabric’ originated from a petrology background where it has been used to describe the arrangement of the constituents of a rock. The association of fabric with soils was first mentioned by Kubiena (1953) and its definition formalised by Brewer and Sleeman (1960) as:

“the physical constitution of a soil material as expressed by the spatial arrangement of the solid particles and associated voids.”

This definition is, however, incomplete since any load-deformation response of a particulate material is not only related to the spatial distribution of its particles and the pore space but also the load displacement behaviour at the inter-particle contacts. Thus, in order to define the structure that is present in a granular mass, one needs to consider the orientation of the inter-particle contact as well as the arrangement of the particle and the associated voids.

Figure 2.1 presents a graphical representation of two idealised soil specimens at the same relative density and identical particle shapes but exhibiting different particle arrangements, i.e., different fabrics.
The terms “fabric” and “structure” will be used interchangeably throughout this thesis.

![Figure 2.1 Two idealised granular medium with identical void ratio but different particle arrangement](image)

**Figure 2.1** Two idealised granular medium with identical void ratio but different particle arrangement

### 2.3. Mechanical implication of fabric

The fabric of granular materials, such as railway ballast, is anisotropic. Within soil mechanics, this anisotropy can be divided into two types. Inherent fabric anisotropy is produced through the depositional process (e.g. sedimentation) and can be defined as a physical characteristic inherent in the soil before any shear strain has occurred. On the other hand, induced fabric anisotropy is the result of non-elastic deformation due to shear strain associated with applied stresses (Razeghi and Romiani 2014; Oda 1993). The mechanical properties of such materials are known to be reliant on the direction of the applied load relative to the material fabric (Tong *et al.* 2014).

Arthur and Menzies (1972) investigated the influence of fabric anisotropy by carrying out (cubical) triaxial element tests on reconstituted sand where the specimen mould was tilted at various angles to the direction of pouring. Arthur and Menzies found a difference of over 200% in the axial strains taken to reach a given stress ratio for sand specimens at the same void ratio and stress level. They also found that specimens prepared at a 90° tilt to the direction of loading was 10% stronger than specimens with a 0° tilt. Similar findings were also reported by Oda (1972b). Oda *et al.* (1982) performed biaxial compression test on specimens that were composed of almost circular rods with aspect ratio of 1:1 and specimens composed of more elongated particles with aspect ratio of 1:4. The specimens were
prepared with the major axis of the particles lying parallel to the bedding plane and bedding angles (θ) of 0°, 30°, 60° and 90° were used. Figure 2.2 shows the peak stress ratio (σ₁/σ₅) plotted against angle θ. Considering the particle geometry it can be seen that for the assembly of elongated particles the strength anisotropy is more pronounced. There is clear evidence of the effect of fabric anisotropy; the stress ratio at failure shows a maximum value for θ = 0°, i.e., major principal stress perpendicular to the bedding plane and a much lower value for θ = 60°.

The effects of soil fabric on the strength of sands have also been documented in laboratory tests where specimens of the same sand, with the same void ratio, were made using different specimen preparation methods. Ibrahim and Kagawa (1991) found that dry air pluviation produced a random particle arrangement that was weak under cyclic shearing. Wet tamping on the other hand, produced a regular particle arrangement that was stronger.

Figure 2.2 Plot of peak stress ratio versus orientation. Specimens with particles almost circular rods (aspect ratio 1.1) is referred to as oval I and the specimen composed of more elongated particles (aspect ratio of 1.4) is referred to as oval II (Oda et al. 1982)
The effects of fabric on natural sand is reported by Cresswell and Powrie (2004) who carried out a series of triaxial compression tests on intact and reconstituted specimens of Reigate silver sand – an inter-locked sand characterised by minimal cement content, large grain contacts, and a relative density index of 136%. Higher peak stress-ratios were observed for the intact soil specimens in comparison with the reconstituted specimens. Additionally, the intact specimens appeared to be slightly stiffer than the reconstituted specimens at larger strains.

Zdravkovic and Jardine (1997) investigated the effect of fabric anisotropy on soil stiffness by performing hollow cylinder apparatus (HCA) tests (and triaxial apparatus tests) on a quartzitic silt. They found that the non-linear stiffness characteristics of the soil are dependent on the stress path direction and the orientation of the major principal stress axis. Kuwano and Jardine (2002) used bender elements, mounted in triaxial apparatus specimens, to measure three types of shear waves \( (S_{dh}, S_{bh}, and S_{hh}) \) in order to investigate the directional dependence of shear wave velocities on sand. Stiffness anisotropy was seen in freshly formed specimens under isotropic confining stresses, reflecting their initially anisotropic (air-pluviated) fabrics. This anisotropy could, however, be accentuated or modified considerably by applying anisotropic effective stress conditions. By conducting similar experiments on specimens of pluviated Toyoura sand and specimens made of rice grains (with an aspect ratio 7:2), Wang and Mok (2008) showed that the inherent stiffness anisotropy is much more pronounced for specimens with elongated grains. Also using bender elements, Ventouras and Coop (2009) demonstrated, in the triaxial tests on Thanet sand, that for large strains the intact soil specimens were stiffer than the reconstituted specimens.

2.4. Observation of fabric

In order to quantify fabric, parameters such as particle orientation and contact normal orientation across an entire specimen needs to be measured. However, the opaque nature of natural granular materials makes this impossible using plain sight. Initially, thin sectioning (where a specimen is fixed by impregnating with resin and then sectioned using a cutting device) offered the only means of investigating the internal structure of a granular material. The use of thin sections
coupled with stills imaging was reported by Oda (1972b) and Oda (1972c) while polished surfaces of resin impregnated specimens were used by Jang and Frost (2000). When stereographic methods are used, 2D images can be the basis to extract 3D quantities (Kuo 1998; Kanatani 1984a). Serial sectioning can also be used to produce 3D datasets. The technique consists of reconstructing a given specimen to a 3D volume by stacking together a series of 2D images taken of the surface after successive removal of thin layers of material from the specimen (e.g., Yang et al. 2008). However, thin sectioning is highly labour intensive and destructive.

Non-destructive techniques include Magnetic Resonance Imaging (MRI) (e.g., Iwashita & Oda 2000; Samieh & Wong 1997), ultrasonic testing and X-ray Computed Tomography (XCT) (e.g., Hasan & Alshibli 2012; Desruies et al. 2010; Wang et al. 2004; Fonseca et al. 2013). The MRI technique makes use of the magnetic properties of hydrogen and its interaction with an external magnetic field to produce 3D images of the internal features of an object. For practical reasons the use of MRI is limited to the application of artificial particles containing mobile hydrogen molecules. Therefore, application to granular soils is only possible on specimens containing interstitial water. XCT like conventional radiography, is based on the attenuation of X-rays following interaction with matter and subsequent tomographic reconstruction of a series of 2D projections (or radiographs) taken from a range of angles. A detailed description of the method will be given in Chapter 3.

2.5. Quantification of fabric

2.5.1. Void ratio

Soil state parameters based on the relationship between the volume of solid particles in the material and the overall volume occupied by the granular material has been used as a basic measure of fabric. The void ratio or \( e \) is perhaps most well-known within geomechanics. It is defined as ratio of the volume of voids \( (V_v) \) to the volume of solid particles \( (V_s) \) such that,
\[ e = \frac{V_v}{V_s} \quad (2.1) \]

Other scalar measurements of the material packing density or fabric include the porosity \( n \), defined as the ratio of the volume of voids to the total volume \( (V_t) \),

\[ n = \frac{V_v}{V_t} \quad (2.2) \]

and specific volume \( v \), the total volume occupied by the material per unit solid volume and is given by

\[ v = \frac{V_t}{V_s} \quad (2.3) \]

However, as they are based on the volume of the different phases of a granular mass they can be described in terms of \( e \),

\[ n = \frac{e}{1 + e} \quad (2.4) \]

\[ v = 1 + e \quad (2.5) \]

Additionally, these metrics quantify the particle packing density of the total mass of particles, without explicitly considering the particulate structure and the natural variation that exists in a heterogeneous material.

2.5.2. Contact coordination number

The contact coordination number \( (CN) \), which reports the number of contacts per particle in the material, is another scalar metric that is used to quantify the state of relative configuration of constituting particles in random granular assemblies. The simplest definition of \( CN \) is

\[ CN = 2 \frac{N_c}{N_p} \quad (2.6) \]

where \( N_c \) is the total number of contacts and \( N_p \) is the number of particles. \( N_c \) is multiplied by 2 as each contact is shared between two particles. With the advent of DEM and a plethora of information on the state of particles, the definition of \( CN \) has been continually refined and redefined. Kuhn (1999) proposed that the effective \( CN \) should include only those particles that participate in the load
bearing matrix of the material. In this case the previous formula for the $CN$ remains the same with the additional condition that only particles with more than two contacts (in 2D) are included in the analysis. Thornton (2000) in essence expressed the same idea of filtering particles (and therefore contacts) based on the number of contacts a particle possesses but with a lower discrimination threshold and called it the mechanical (contact) coordination number

$$mCN = 2 \frac{N_c - N_1}{N_p - N_0 - N_1}$$  \hspace{1cm} (2.7)

where $N_0$ and $N_1$ are the number of particles with zero and one contact respectively. It should be noted that the $CN$ is calculated for a given instant in time and particles that may have been filtered out in one instance may later be included as deformation takes place.

It seems logical to link changes in $CN$ to the void ratio since intuition would suggest that an inverse relationship exists between them. Thus, a number of different expressions relating the coordination number to the void ratio have been proposed based on experimental studies on spheres (e.g., Oda 1977; Rowe 1962; Chang et al. 1989; Mitchell & Soga 1976; Field 1963). However, others such as Rothenburg and Kruyt (2004) and Hasan and Alshibli (2010) have shown that empirical relationships between particle contacts and volume change may not be appropriate as they have been developed using regular packing of rigid and equal sized spheres.

2.5.3. The fabric tensor

The fabric tensor $F$ is perhaps the most widely used metric in quantifying the fabric (or anisotropy) that exists in a granular mass. At its simplest, the fabric tensor is a second order tensor that provides a means of conveniently averaging orientation vectors thus allowing the determination of the preferred orientation and the magnitude of the anisotropy. The averaging can be performed on either the orientation of major axis of the particles or voids or the orientation of the contact normals between two particles (Figure 2.3).
The most commonly used formulation of the fabric tensor is the one generally attributed to Satake (1976; 1982). In tensorial notation the second-order fabric tensor (for particle orientations in this case) is given as

\[ \mathbf{F}_{ij} = \frac{1}{N_p} \sum_{k=1}^{N_p} n_i^k n_j^k \]  

(2.8)

where \( n_i^k \) is the unit orientation vector for the \( k \)th particle in \( N_p \) number of particles in the specimen. The orientation vector of the \( k \)th particle can be represented in Cartesian/spherical coordinate system such that,

\[ n^k = \begin{pmatrix} n_x^k \\ n_y^k \\ n_z^k \end{pmatrix} = \begin{pmatrix} \sin\psi^k\cos\theta^k \\ \sin\psi^k\sin\theta^k \\ \cos\psi^k \end{pmatrix} \]  

(2.9)

where \( \psi \) and \( \theta \) are inclination (zenith) and azimuth angles (to a chosen reference axis) associated with the vector \( n^k \). The \( \mathbf{F} \) for void space orientation or particle contact orientation can be obtained by substituting the relevant unit vectors into Equation 2.8. Expanding Equation 2.8 using a Cartesian coordinates system in 3D gives,

\[
\begin{bmatrix} F_{11} & F_{12} & F_{13} \\ F_{21} & F_{22} & F_{23} \\ F_{31} & F_{32} & F_{33} \end{bmatrix} = \frac{1}{N_p} \begin{bmatrix} \sum_{k}^{N_p} n_x n_x & \sum_{k}^{N_p} n_x n_y & \sum_{k}^{N_p} n_x n_z \\ \sum_{k}^{N_p} n_y n_x & \sum_{k}^{N_p} n_y n_y & \sum_{k}^{N_p} n_y n_z \\ \sum_{k}^{N_p} n_z n_x & \sum_{k}^{N_p} n_z n_y & \sum_{k}^{N_p} n_z n_z \end{bmatrix}
\]  

(2.10)

The right hand matrix is sometimes referred to as the orientation tensor (Scheidegger 1965). Using spherical coordinate system gives,

\[
\begin{bmatrix} F_{11} & F_{12} & F_{13} \\ F_{21} & F_{22} & F_{23} \\ F_{31} & F_{32} & F_{33} \end{bmatrix} = \frac{1}{N_p} \begin{bmatrix} \sum_{i}^{N_p} \sin^2\psi \cos^2\theta & \sum_{i}^{N_p} \sin^2\psi \cos\theta \sin\theta & \sum_{i}^{N_p} \sin\psi \cos\psi \cos\theta \\ \sum_{i}^{N_p} \sin^2\psi \cos\theta \sin\theta & \sum_{i}^{N_p} \sin^2\psi \sin^2\theta & \sum_{i}^{N_p} \sin\psi \cos\psi \sin\theta \\ \sum_{i}^{N_p} \sin\psi \cos\psi \cos\theta & \sum_{i}^{N_p} \sin\psi \cos\psi \sin\theta & \sum_{i}^{N_p} \cos^2\psi \end{bmatrix}
\]  

(2.11)

The sum of the diagonal elements or trace of the fabric tensor is always 1 (i.e. \( F_{11} + F_{22} + F_{33} = 1 \)). Further, since this second order tensor is symmetric i.e. \( F_{ij} = F_{ji} \).
the three principle values ($F_1$, $F_2$ and $F_3$) are real and the three principal directions (1, 2, and 3) can always be found.

![Figure 2.3 Illustration showing a 2D schematic definition of the major axis of a particle and the contact normal used for fabric analysis.](image)

**Figure 2.3** Illustration showing a 2D schematic definition of the major axis of a particle and the contact normal used for fabric analysis.

![Figure 2.4 Three different idealised granular assemblies where particles are oriented at (A) 0°, (B) 90° and (C) 60°.](image)

**Figure 2.4** Three different idealised granular assemblies where particles are oriented at (A) 0°, (B) 90° and (C) 60°.

Consider the idealized granular assemblies in Figure 2.4 where all the particles are aligned parallel to the $xz$ plane so that the $y$ component is always zero. In assembly A, all the particles are aligned with the horizontal giving an identical orientation vector for all particles such that,
\[ n^{1-6} = \begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \]  
(2.12)

Applying Equation 2.8,

\[
\mathbf{F}_{ij}^A = \frac{1}{6} \begin{bmatrix}
(1 \cdot 1 + \ldots + 1 \cdot 1) & (1 \cdot 0 + \ldots + 1 \cdot 0) & (1 \cdot 0 + \ldots + 1 \cdot 0) \\
(0 \cdot 1 + \ldots + 0 \cdot 1) & (0 \cdot 0 + \ldots + 0 \cdot 0) & (0 \cdot 0 + \ldots + 0 \cdot 0) \\
(0 \cdot 1 + \ldots + 0 \cdot 1) & (0 \cdot 0 + \ldots + 0 \cdot 0) & (0 \cdot 0 + \ldots + 0 \cdot 0)
\end{bmatrix}
\]  
(2.13)

\[
\mathbf{F}_{ij}^A = \frac{1}{6} \begin{bmatrix}
6 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{bmatrix} = \begin{bmatrix}
1 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{bmatrix}
\]

The zero off-diagonal terms reveal that the principal direction of assembly A is aligned with one of the axis while the zero diagonal terms confirm that the dominant axis is the \( x \) axis.

Similar treatment of assembly B, where 50\% of the particles have been rotated by 90\°, gives,

\[
\mathbf{F}_{ij}^B = \begin{bmatrix}
0.5 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0.5
\end{bmatrix}
\]  
(2.14)

while with assembly C, where all the particles are oriented at 60\° from the horizontal, the fabric tensor is,

\[
\mathbf{F}_{ij}^C = \begin{bmatrix}
0.75 & 0 & 0.43 \\
0 & 0 & 0 \\
0.43 & 0 & 0.25
\end{bmatrix}
\]  
(2.15)

**Interpreting the fabric tensor**

The fabric tensor is an abstract concept similar to the well-known stress tensor. The principal stresses and their orientations can be determined from the stress tensor by solving the eigenvalue problem. Similarly, eigenvalue decomposition of the fabric tensor will give the preferred orientations and the magnitude of the anisotropy within a granular system.

The eigenvalue problem is to determine the nontrivial solutions of the equation,
\[ A \hat{\mathbf{v}} = \lambda \hat{\mathbf{v}} \]  

(2.16)

where \( A \) is an \( n \)-by-\( n \) matrix, \( \hat{\mathbf{v}} \) is a column vector of length \( n \), and \( \lambda \) is a scalar. The values of \( \lambda \) that satisfy the equation are the eigenvalues. The corresponding values of \( \hat{\mathbf{v}} \) that satisfy the equation are the right eigenvectors. The magnitude of the major fabric is given by \( \lambda_1 \), the intermediate fabric is given by \( \lambda_2 \) and the minor fabric is given by \( \lambda_3 \) (i.e. \( \lambda_1 > \lambda_2 > \lambda_3 \)). The eigenvalues have the property of \( \lambda_1 + \lambda_2 + \lambda_3 = 1 \), and are a measure of the degree of clustering data from the respective eigenvectors.

A fully anisotropic fabric will be manifested by three distinct eigenvalues, while a transversely anisotropic or cross-anisotropic fabric will yield only two distinct eigenvalues.

The extent of the bias in the most preferential direction of fabric orientation is given by the largest eigenvalue and the corresponding eigenvector gives the direction of the principal fabric component. Thus, for example, the eigenvalues for the fabric tensor of assembly \( C \) (i.e. Equation 2.15) are,

\[
\begin{pmatrix}
\lambda_1 & 0 \\
\lambda_2 & 0 \\
\lambda_3 & 1
\end{pmatrix}
\]  

(2.17)

and the eigenvector associated with \( \lambda_3 \) is,

\[
\hat{\mathbf{v}}_3 = \begin{pmatrix} 0.866 \\ 0 \\ 0.500 \end{pmatrix}
\]  

(2.18)

Converting the eigenvector into angles gives an inclination angle of 60°.

While it is accepted that the principal components of fabric, \( \lambda_1 \), \( \lambda_2 \), and \( \lambda_3 \) can be used to describe the intensity of the anisotropy, different formulations have been proposed. Some authors suggest that the difference between the major and intermediate eigenvalues (i.e. \( \lambda_1 - \lambda_2 \)) is an appropriate measure of the structural anisotropy. This is sometimes known as the deviator fabric (e.g, Thornton 2000). Maeda (2009) described the use of a slightly different form of the deviator fabric, which he calls the “deviator fabric intensity”, this is given as the product of the
coordination number and the deviator fabric, i.e. $CN(\lambda_i - \lambda_d)$. Instead of looking at the difference between the principal eigenvalues of the fabric tensor, some authors have considered the ratio of these two components. For example, Wan et al. (2005) and Ibraim et al (1991) quantified anisotropy as the ratio of the major and minor eigenvalues (i.e. $\lambda_i/\lambda_d$).

The measures outlined above are designed for two-dimensional systems or three-dimensional transversely anisotropic (cross-anisotropic) systems and so the intermediate fabric component is neglected.

Kuo et al. (1998) and Barreto et al. (2009) considered more general formulations to include the intermediate fabric component ($\lambda_d$). They proposed quantifying the 3D anisotropy or deviator fabric using the following invariant (analogous to the shear stress in the octahedral plane):

$$\lambda_d = \frac{1}{\sqrt{2}} \sqrt{(\lambda_1 - \lambda_2)^2 + (\lambda_2 - \lambda_3)^2 + (\lambda_3 - \lambda_1)^2} \quad (2.19)$$

Woodcock (1977) presented a graphical technique to interpret the fabric eigenvalue data by plotting $\ln(\lambda_i/\lambda_d)$ versus $\ln(\lambda_d/\lambda_d)$. This is illustrated in Figure 2.5. Woodcock also defines two distribution indicators (or fabric descriptors),

$$\beta_1 = \frac{\ln(\lambda_1)}{\ln(\lambda_2/\lambda_d)} \quad (2.20)$$

$$\beta_2 = \ln(\lambda_1/\lambda_d)$$

where $\beta_1$ and $\beta_2$ are the shape factor and the strength factor respectively. For an isotropic fabric the eigenvalue data are uniformly distributed and plots at the origin. If on the other hand the fabric is anisotropic, the shape factor $\beta_1$ will indicate the extent of the concentration of vectors in the preferred orientation and the strength factor $\beta_2$ will determine whether the distribution of orientations is a cluster or a girdle. Also, in the case of an axisymmetric fabric (i.e. $\lambda_2 = \lambda_3$) the eigenvalue data will plot along the vertical axis.
Figure 2.5 Two-axis logarithmic plot of ratios of normalized eigenvalues (after Woodcock 1977)
2.6. Particle shape.
Shape of ballast aggregate is one of the most important factors to affect ballast strength, workability, and stability. However, compared to particle gradation and air voids, the influences of aggregate shape properties on aggregate assembly strength, stability, and deformation characteristics have received less attention and have not been thoroughly investigated by means of quantifying individually the effects of aggregate morphological properties on the mechanics and fabric of a ballast bed.

2.6.1. Effects of particle size and shape

Particle size
The particle size and its distribution (or grading) has been traditionally identified as one of the most important factors affecting the behaviour of a granular media. Particle size gradation greatly influences the overall packing and void ratio. The possible range of packing of soil particles is often related to the maximum and minimum void ratios, reflecting the loosest and densest states respectively. Well graded soils have low void ratios compared with more uniform soils, because the smaller particles fill the large voids enclosed by large particles (Miura et al., 1997). In addition, the void ratio range ($e_{\text{max}} - e_{\text{min}}$), has been found to be dependent on the grain size distribution (Miura et al. 1997; Cubrinovski & Ishihara 2002). Figure 2.6 shows that the void range decreases as $d_{50}$ increases.

![Figure 2.6 Change in void ratio with mean grain size (Miura et al. 1997)](image-url)
Figure 2.7 Comparison of stable (a) and unstable contacts (Yamamuro & Wood 2004)

The distribution of particle sizes influences the soil response, for example, at the same relative density a better graded soil may have a larger angle of internal friction (e.g., Huffine and Bonilla, 1962). In addition, previous studies have also suggested the effect of particle size in the compressibility of granular soils. Huffine and Bonilla (1962) showed that finer soils tend to be more compressible. Yamamuro and Wood (2004) demonstrated that soils with a wide range of particle sizes are likely to create a more compressible soil skeleton in comparison with soils with a narrower particle size distribution. The authors attributed this to the occurrence of unstable contacts formed by large-to-small-to-large (L-s-L) grains. Figure 2.8a shows that contacts formed by large-to-large (L-L) particles were associated with more stable responses while unstable contacts appear to be related to soil liquefaction (Figure 2.7b).

**Particle shape**

However, when the PSD is similar, particle shape has been shown to alter the response of granular soils dramatically.

Koerner (1970) investigated the effects of particle shape on the shear strength of granular soils by performing drained triaxial compression tests at different densities on angular, sub-angular and sub-rounded crushed quartz and Ottawa
sand (Figure 2.8). Koerner’s results showed that as particle shapes changed from sub-rounded to angular; the angle of shearing resistance saw significant increase (Figure 2.9). Chern (1985) showed that, at equal relative densities, angular sand was more resistant to liquefaction at lower confining pressures but less resistant at higher confining pressures than rounded sand. Selig and Roner (1987) concluded that the strength of a granular material is affected by the inclusion of flat/flaky or other extreme dimensional measurement material such as elongated particles. Shahu and Yudhbir (1998) carried out model plate load tests, model standard penetration tests and direct shear tests on three angular compressible natural sands and one rounded sand. Their results show that at a given relative density the angular sands outperform the rounded sand in all tests i.e. the angular sand blow count in the model standard penetration test, failure load in the model plate load test and angle of shearing resistance were much higher. Guo and Su (2007) performed drained triaxial compression tests on two sands at different confining pressures and initial void ratios and showed that inter-particle locking due to the angularity of particles tends to increase the peak friction angle and affects the dilatancy characteristics of sand. Similar observations, regarding the increase of shearing resistance with increasing particle angularity, were made by Alshibli and Sture (2000), Shinohara et al. (2000), Sukumaran and Ashmawy (2001), Mair & Frye (2002), Liu and Matsuoka (2003), and Rouse et al. (2008). A review by Cho et al (2006) of their experimental data and results from published studies showed that as roundness and sphericity decreased, an increase in $\epsilon_{\text{max}}$ and $\epsilon_{\text{min}}$ was measured. Furthermore, Cho et al showed that at small strains, specimens consisting of highly irregular particles have reduced stiffness, increased compressibility and an increased angle of friction at steady state shearing. Using a hollow cylinder apparatus Tsomokos and Georgiannou (2010) examined the undrained response of four sands (two angular and two rounded) to torsional shear at various stress levels and densities. They observed that sands with rounded grains underwent systematic weakening or shear stress reduction after a transient peak deviator stress. However, angular grained sands with the same grading curve and void ratio, showed stable response with a continuous increase in strength after a transient peak.
As with the study of fabric, DEM has facilitated a greater understanding of particle shape and its influence on granular mechanics. Rothenburg and Bathurst (1992) performed 2D numerical simulations of biaxial compression tests on discs and elliptical particles. Their results showed that as particle shapes deviated away from a perfect disc, initial CN increased and consequently increased peak and critical state strength. Mirghasemi et al (2002) used DEM simulations on assemblies of 2D polygon shaped particles (Figure 2.10) to show that the peak shear strength of angular materials occurred at a higher axial strain than that of
materials having rounded particles, with a less significant reduction in post-peak strength. Mirghasemi et al. concluded that both the shear strength and dilation increased with particle angularity, which substantially restrained particle rotation during deformation. Similar work was performed by Pena et al. (2006), who explored the influence of particle shape on the mechanical behaviour of two-dimensional particle assemblies comprising grains of randomly generated convex polygons. They noted that the average accumulated particle rotation was substantially lower for elongated particles than that for particles whose aspect ratio was unity. Lu and McDowell (2007) carried out comparative 3D sleeper box tests on clumps of spheres (e.g. Figure 2.11) and spheres. They showed that the angularity vastly reduced particle rotation and spatial displacement under loading.

![A 100 sphere clump](image)

Figure 2.11 A 100 sphere clump (Ferellec & McDowell 2010)

### 2.6.2. Description of shape

Particle shape and its quantification have been given constant attention in the literature for nearly a century tracing back to the early work of Wentworth (1919) on cobble abrasion. Since then countless metrics have been devised to quantify shape. At the same time, the aspects and terminologies associated with shape have also been debated without consensus amongst the research community and continue today.
In this work, the different descriptors of shape will be described in line with the definition put forward by Griffiths (1967) and popularised by Barrett (1980). Form, a first order shape parameter, is defined as the combination of element that affects the 3 dimensional (3D) proportions of the particle. Angularity is a second order parameter which describes the geometrical configuration of the surface envelope of the particle. Roughness, a third order parameter, is the surface irregularity present on the particle and usually simplified to surface friction. A graphical definition of the descriptors is presented in Figure 2.12, while alternative terminology for these definitions is given in Table 2.1.

![Diagram of Form, Angularity, and Roughness](image)

*Figure 2.12 Schematic definition of Form, Angularity and Roughness (after Barrett 1980)*

<table>
<thead>
<tr>
<th>Order</th>
<th>Shape Characterise</th>
<th>Alt. term</th>
</tr>
</thead>
<tbody>
<tr>
<td>1st</td>
<td>Form</td>
<td>Sphericity</td>
</tr>
<tr>
<td>2nd</td>
<td>Angularity</td>
<td>Roundness</td>
</tr>
<tr>
<td>3rd</td>
<td>Roughness</td>
<td>Surface texture</td>
</tr>
</tbody>
</table>

**Form**

Form is normally measured as a ratio based on the longest (L), smallest (S) and intermediate (I) orthogonal axes of a particle. A ratio is most suitable as it allows comparisons to be made irrespective of particle size (Barrett, 1980).
Amongst the first to quantify particle form using a combination of the three orthogonal dimensions was Wentworth (1922a) with his Flatness index,

\[
\text{Flatness Index} = \frac{L + I}{2S}
\]  

(2.21)

Zingg (1935) used L, S, and I of a particle to calculate two simple ratios:-

\[
\text{Elongation} = \frac{S}{I}
\]  

(2.22)

\[
\text{Flatness} = \frac{I}{L}
\]  

(2.23)

These were then plotted on a bivariate graph (Figure 2.13), segmented at a ratio of 2:3, allowing form to be classified as ‘flat’, ‘spherical’, ‘flat and columnar’ and ‘columnar’.

Wadell (1935) developed the concept of sphericity as an aspect of form. Wadell suggested the use of a sphere as a reference form and considered that deviations (of the particle form) were best represented by ratios of particle volume to the volume of the circumscribed sphere. This is calculated using:-

\[
\text{Wadell’s Sphericity} = \sqrt[3]{\frac{\text{Volume of particle}}{\text{Volume of circumscribing sphere}}}
\]  

(2.24)

Wadell’s approach measures the deviation of a particle’s form from that of a sphere. However, it was seen that by rounding the edges of a cube, the Wadell sphericity of the cube would change proving that Wadell’s measure was not exclusive to form alone but also had an element of angularity.

Krumbein (1941) took a more holistic approach and combined Zingg’s flatness index with Wadell’s sphericity. Krumbein also changed the reference form to an ellipsoid as a better approximate to rock particles.

The equation he derived, called the intercept sphericity (IS), was a function of the volume ratio of the ellipsoid as defined by the three axes to the circumscribing sphere within a particle.
2. Literature review

\[
\text{Intercept Sphericity (IS)} = \sqrt[3]{I \times S \over L^2}
\]  \hspace{1cm} (2.25)

This parameter had the advantage over Wandells’ sphericity of being an exclusive measure of form.

Sneed and Folk (1958) also suggested a similar measure to Krumbein’s Intercept Sphericity. Sneed and Folk argued that the sphericity of a particle should express its behaviour in a fluid as they tend to orientate themselves with the maximum projection area normal to the flow. They derived a ratio between a sphere of equal volume to the particle and a sphere with the same maximum projection area. The Maximum Projection Sphericity (MPS), as it is known, can be calculated from,

\[
\text{Maximum Projection Sphericity} = \sqrt[3]{S^2 \over I \times L}
\]  \hspace{1cm} (2.26)

However, a major drawback of this measure is its dependence on the dynamic behaviour of the particle in a fluid medium. Thus, in a situation where this behaviour is unimportant, the maximum projection sphericity may be inappropriate.

It is interesting to note that Sneed and Folk’s measure of sphericity is very close to that of Krumbein’s intercept sphericity, i.e. maximum projection sphericity uses the shortest axis (S) as a reference while the intercept sphericity uses the longest axis (L).

![Figure 2.13 Zingg’s diagram](image-url)
**Angularity**

The most commonly used measure of angularity is that described by Cox (1927) which he calls ‘percentage roundness’. Since then this measure has been used by many researchers (Wheless *et al.* 1994; Pambuccian *et al.* 1997; LoPachin *et al.* 2003; Nafe *et al.* 2006; Foresto *et al.* 2000). The percentage roundness (PR) is best described as the ratio of the area of the object to the area of a circle with the same perimeter as the object. However it is equivalent to the ratio of the respective perimeters:

\[
PR = \frac{A}{A_p} = \frac{4\pi A}{P^2}
\]  

(2.27)

where \(A\) is the area of the object, \(A_p\) is the area of a circle with the same perimeter as the object and \(P\) is the object’s perimeter. Percentage roundness for all objects lies in the range of 0 to 1, with only a circle giving the highest value of 1. Derivations of this measure are also proposed in the literature, often described as if they were new measures. Richardson (1961) defines ‘homoplaty’ as

\[
H = \frac{2\sqrt{\pi A}}{P}
\]  

(2.28)

However, this is the square root of the percentage roundness. The additional square root calculation adds no more than a nonlinear scaling of the percentage roundness.

Foresto *et al.* (2000) define the ‘aggregate shape factor’ as

\[
ASF = \frac{A}{P^2}
\]  

(2.29)

This measure is a non-normalised version of the percentage roundness. In effect this means that its range is 0 to \(4\pi\), which is a less intuitive range than the normalised version.

Diamond *et al.* (1982) defined a measure they call the ‘nuclear roundness factor’:
\[ NRF = \frac{r_p}{r_a} \]  \hspace{1cm} (2.30)

where \( r_p \) is the radius of a circle with the same perimeter as the object, and \( r_a \) is the radius of a circle with the same area.

However it can be shown that,

\[ NRF = \sqrt{\frac{1}{PR}} \]  \hspace{1cm} (2.31)

Therefore this proposed measure is in fact the inverse square root of the percentage roundness.

Hausner (1966) defines a measure he calls “surface factor”.

\[ SF = \frac{P^2}{4\pi A} \]  \hspace{1cm} (2.32)

This is an inverse of the percentage roundness and is also used by others (Jayaraj et al. 2005; Dell’Aquila 2004; Kanthathas et al. 2005). This measure has the disadvantage that its range is in fact 1 to infinity, where a circle has a value of 1.

Moschakis et al. (2005) divide the surface factor by 1.064 to compensate for the square corners produced by digitization

\[ Moschais\ Roundness = \frac{P^2}{4\pi A \cdot 1.064} \]  \hspace{1cm} (2.33)

As stated previously, the percentage roundness and its mathematical derivations have been widely used. However Richardson (1961) mentioned (and later Mandelbrot (1967) showed) that the perimeter of a shape increases as the unit of measure decreases. Increasing the resolution of an image is equivalent to reducing the unit of measure, and hence one could expect the perimeter to grow non-linearly with increased resolution.
2.7. Summary

This chapter has reviewed, relevant literature in two broad areas; the effects of shape on the mechanical response of un cemented granular media and the fabric that develops in them.

A substantial body of literature exists on the laboratory investigation of fabric in granular media. This clearly shows that the mechanical response observed in such materials is (significantly) influenced by the interlocking of the individual particle, i.e. fabric. This has greatly encouraged research into fabric measurement techniques. While there are now a number of methods for the observation of fabric, the application of X-ray Computed Tomography (XCT) has been the most productive. However, all available studies into fabric using XCT have been carried out on sands or other materials consisting of sub-millimetre sized particles.

A similar paradigm is observed when parameterisation of particle shape is considered in numerical models. Laboratory experiments show that particle shape influences the mechanical behaviour of granular materials. Even so, numerical models tend to oversimplify particle geometry for the benefit of expediency over accuracy.
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3

Analysis of fabric in railway ballast using X-ray CT

3.1 Introduction

The fabric of a granular material, such as the ballast bed of a railway track, plays an important role in its response to loading. Over its life, the fabric or internal structure of the ballast bed may change in response to external factors such as trafficking and maintenance. A better understanding of ballast mechanics is needed to facilitate the cost effective maintenance of existing railways and inform the design of new high speed tracks.

The study of fabric in granular media has traditionally been carried out by analysing photographs of (serial) thin sections taken either horizontally or vertically through a specimen impregnated with a bonding agent (e.g. Parkin et al. 1968; Oda, 1972a). However, this method is destructive, prone to errors associated with inconsistent sectioning and tends to be highly labour intensive.

With recent advances in industrial X-ray computed tomography (XCT) technology, its use in the field of geomechanics is increasing rapidly as a replacement for thin sectioning and photoelastic materials. The use of this technology in the geomechanics community has been mainly focused on fine grained (sub-millimetre scale) materials such as sands (e.g. Oda et al, 2004) while gravel sized materials such as ballast have been largely ignored. This has been
primarily due to the difficulty in CT scanning large specimens consisting of dense materials that the X-rays are not able to penetrate. As a result, fabric in large scale granular systems remains unexplored. More specifically, unbonded gravel sized granular media such as ballast pose two substantial challenges that have yet to be addressed:

1. How to retrieve a specimen from underneath the rail seat (shown hatched in Figure 3.1) with its fabric intact under field conditions
2. How to CT scan a specimen that has a nominal diameter of at least 300mm and consists of highly dense rock packed very closely

In this chapter, a novel technique for retrieving intact specimens from ballasted railway tracks is described and implemented in the field.

Then, cutting-edge CT technology is used to develop scanning protocols that allow high resolution 3D imaging and subsequent analysis of these specimens and their fabric.

![Figure 3.1. Illustration of a typical ballasted railway track cross section showing the location where the sampling is performed.](image)
3.2. Fabric intact sampling of railway ballast

Undisturbed sampling techniques form an important part of laboratory testing and analysis on a variety of aspects of soils (e.g., strength, hydraulic conductivity, etc.). Various methods have been developed for intact sampling of cohesive soils (e.g., Brown et al. 1985; Buchter et al. 1984; Economy & Bowman 1993) and locked sands (Cresswell 2001) where segregation is not an issue when carefully handled. Sampling of cohesion-less granular media with its fabric or structure intact is also common place amongst experimentalists working with sands and other fine grained materials within the laboratory environment (e.g., Oda et al. 2004; Fonseca et al. 2012).

In the field, ground freezing techniques have been used for the recovery of intact sand specimens over a number of decades (e.g., Hofmann et al. 2000). However its applicability to larger grain sized materials such as ballast has not been demonstrated. The use of resins or glues to preserve fabric in specimens has been documented over the past few decades. Klassen et al. (1987) used epoxy resin to preserve laboratory-prepared specimens of railway ballast and carried out mechanical sectioning of these specimens, which were then evaluated qualitatively in terms of particle interlocking and void characteristics for different gradations. However, few if any attempts have been made to use resins or glues to recover fabric preserved field specimens.

3.2.1. Sampling methodology

The method described here is conceptually similar to existing resin/glue based sampling techniques where by a binding agent is used to encase a volume of ballast approximately 300mm × 300mm × 300mm directly beneath the sleeper railseat (Figure 3.1) and subsequently remove it.

In reality the process is significantly complicated by two factors; the sampling has to be carried out on functioning railways lines; and the mass of the final specimen can be in excess of 80 kg. Furthermore, the viscosity and curing time of the resin, as well as the quantity used, must satisfy conflicting requirements. The resin must be fluid enough to move through the voids in the ballast layer, but viscous enough
not to disperse too far below the intended sampling depth before curing to a strength sufficient for specimen removal. The curing time should be as short as possible to minimize disruption to operation railway lines, but long enough for the resin to reach the required depth.

Preliminary tests on laboratory specimens (using full sized ballast) showed that polyurethane resin EL366D/NC (Robnor resins 2013) mixed with a chalk filler to increase viscosity satisfies these requirements. At 25°C it has an initial viscosity without filler of less than 200 mPa and a useable time of 2 minutes. Specimens have been obtained at temperatures as low as 5°C. While there are probably a number of resins that would be suitable for the sampling process the main advantage of resin EL366D/NC over other resins trailed was the short cure time, which was key to sampling on operational lines during planned overnight maintenance works. The resin is also advertised as having very low shrinkage (Robnor resins 2013). The resin was supplied by Robnor in 2 kg kits consisting of 1 kg of resin and 1 kg of hardener to be mixed together (data sheets are available from (Robnor resins 2013)). The chalk was also supplied by Robnor in 3 kg tubs. The quantity of chalk used varied but may be estimated as approximately 1/4 of the final mixture by weight.

Given the weight of individual specimens, a method to lift the specimen has also been developed whereby a metal grid with lifting eyelets is bonded to the top of the specimen (i.e. by pouring the resin through it) and recovered using a mechanical lifter. Additionally the framing metalwork of the grid was made from L-section bars that help control the pouring area, hence the size of the final resin bulb (Le Pen et al. 2014).

A point of concern with any resin based sampling technique is the expansive/contractive potential of the materials used. Initial trials showed that the resin mixture is susceptible to visible expansion under certain conditions where air bubbles trapped in mixtures with high filler content (and therefore higher initial viscosity) expand due to the heat generated during the curing process. This however is not detrimental since the curing mixture remains adequately fluid for any expanding resin to travel into the large void space present
in the ballast bed. Subsequent CT scans and mechanical slices along the specimen edges show that particles are in contact demonstrating that there is no observable disturbance on the fabric. Observation of the curing process on site indicated no uplift around the sampling locations, perhaps aided by the well compacted and horizontally confined nature of the ballast being sampled. It is also worth noting that the resin only bonds weakly with the ballast particles (which are usually damp and coated in dirt), with specimen integrity maintained primarily by the cross linked resin-filled network of voids. This last observation is consistent with the mechanism of support commonly associated with ballast gluing for track remediation.

A summary of the method is as follows (after Le Pen et al. 2014):

- A metal lifting/resin entry grid, measuring 200 mm², is placed onto the cleared ballast surface beneath the sleeper railseat (Figure 3.2)
- The resin is prepared in a bucket using a cordless drill with a stirring bit. It is first mixed with a chalk filler, normally as much as the resin will accept, to increase its viscosity. The hardener is then added, giving the mixture a treacle-like consistency. More chalk filler may be added but this is not usually necessary. Up to 8 kg of resin/hardener are needed, typically delivered in 2 to 3 pours, each being a separately prepared mixture. The first pour will consist of a 2 kg resin/hardener kit with chalk filler added, the second pour will be twice this quantity (4 kg+chalk filler) and the last pour (if needed) is a further 2 kg kit with chalk filler. This spacing of the pours allows the resin to cure sequentially and helps control the size of specimen obtained with the initial pours coating the particles and closing off the voids by curing giving the later pours less freedom to flow out of the intended specimen volume.
- After the resin has cured sufficiently (evaluated by timing, visual inspection and touch, and allowing some additional time for conservatism) the material around the resin bulb is excavated using a shovel to reduce resistance to lifting (Figure 3.3 top).
• The specimen is removed using a mechanical lifter, e.g. a Rail Road Vehicle (RRV) (Figure 3.3B) within 30 minutes of the first pour.
• The specimen is placed in a container and transported to the laboratory (Figure 3.3 bottom).
• At the laboratory the specimen is placed into a plastic box and sealed by pouring more resin around it. The entry grid is levered off. The specimen is then cut to a suitable shape, using a diamond saw (Figure 3.4).

3.2.2. Large scale specimens
The above method has been successfully applied to three sites in Hampshire, U.K. and one in Tuxford, U.K.

Individual specimens were taken from Arundel (ARU), New Milton (NWM) and Camberley (CAM). The ballast condition at the time of sampling was similar in all three locations. The ballast had been in service nearly 30 years and was considered ready for renewal. Three further specimens were retrieved from Network Rail’s (NR) test facility in High Marnham (HMA), Tuxford. The main track, opened in 2009, is approximately 23 km in length with a design speed of 120 km/h. The track condition at the time of sampling was very good since it had been renewed recently. Out of the six field specimens retrieved in total, four were selected for X-ray CT inspection (Table 3.1 and Figure 3.4).

Two further specimens were prepared in the laboratory, one with zero loading history and the other retrieved from the Southampton Railway Testing Facility (SRTF) shown in Figure 3.5. A detailed description of the apparatus can be found in Le Pen and Powrie (2011). The Loose specimen was prepared by pouring NR specification ballast into a cylinder which was then lightly agitated to stabilise any loose particles that could otherwise move during scanning. No resin was used in this case. The specimen from the SRTF (LRig) also consisted of NR specification ballast which however had been subjected to 3 million load cycles amounting to approximately 60 million tonnes cumulative axle load. The load cycles were divided into three equal stages with stoppages in the middle for data collection. The sampling method described in Section 3.1.1 was used to retrieve a specimen from under the rail seat (Figure 3.5). The ballast used for these
specimens complies with BS EN 13450:2002 grading category A and was sourced from Cliffe Hill quarry, Nottinghamshire, UK.

Figure 3.2 Top: 200mm×200mm lifting grid placed on the ballast heap before the resin in poured. Middle: lifting grid placed on ballast under sleeper seat. Bottom: first batch of resin being poured.
Figure 3.3 Top & Middle: specimen being lifted by excavator. Bottom: sampling complete
Figure 3.4 Field specimens reshaped to octahedrons. A: Arundel (ARU), B: New Milton (NWM), C: Camberly (CAM) and D: High Marnham (HMA).
Figure 3.5 Left: Southampton axel load simulator (LRig). Right: A fabric intact L Rig specimen
3.2.3. Laboratory element test specimens

In order to investigate loading-related changes in the fabric of granular media, triaxial specimens of aggregates were preserved following prescribed loading regimes (e.g., Figure 3.6).

Three large scale drained triaxial tests were carried out on 1/3 scale ballast (BS EN 13450:2002 grading category A reduced by a factor of 1/3 sourced from Cliffe Hill quarry) by Aingaran (2014).

The triaxial apparatus used in the laboratory tests can accommodate a specimen of 150 mm diameter and 300 mm height. The apparatus was supplied by GDS instruments and is described as a 50 kN/1700 kPa load frame-based triaxial testing system in which the ram load $q$ and confining/cell pressure $\sigma_3$ can be independently cycled (GDS 2014). The maximum particle size in the scaled ballast specimen is 22.4 mm resulting in a specimen diameter to particle size ratio that is under the accepted minimum of 1/6 (Indraratna et al. 1993; Marachi et al. 1972).

The triaxial specimens were prepared within a split mould in three consecutive layers. Following standard triaxial testing methods, the tested material is contained within a rubber membrane with porous disks at the top and bottom ends. Each layer was vibrated for one minute under its own weight, and then for a further minute under a 5 kg mass. After placing and vibrating the third layer, the upper surface of the specimen was levelled by manual placement of individual particles up to the top of the mould, followed by further vibration under self-weight. An equal amount (by weight) of scaled ballast is used in each of the three layers in order to achieve similar density throughout the specimen (Aingaran 2014.)

Three different cyclic loading regimes on three separate specimens were tested; compression only, compression – extension and compression – extension – compression (Aingaran 2014).

- Cyclic compression (T1) - the specimen was loaded by cycling the deviator stress and the confining stress (Table 3.3). The loading was one way such
that $q$ was positive throughout the test. The specimen experienced a cumulative axial shortening of 10.20 mm at the end of the test. The specimen went through a total of 1000 cycles.

- Cyclic compression and extension (T2) - the specimen was first loaded as previously described, followed by the reversal of the applied stress through cyclic extension loading (i.e. radial stress $\sigma_r >$ axial stress $\sigma_a$) at a net axial stress of 50 kPa. This was done to simulate track tamping.

- Cyclic compression – extension – compression (T3) – the specimen was first loaded by cycling the deviator stress only. The confining stress remained constant and the specimen went through a total of 1000 cycles in this stage (Table 3.3), followed by extension at a net axial stress of 60 kPa. Finally, the specimen was compressed until the axial displacement was equal to the pre-extension level. This took 1600 cycles of cyclic compression.

The intended stress paths followed by the different triaxial tests are presented in Figure 3.7. The Average effective stress $p'$ is calculated by assuming that $\sigma' = q + \sigma'$ and $\sigma'' = \sigma''$. The bulk densities and void ratios for the resin impregnated triaxial specimens are given in Table 3.2, while the loading stages and the associated testing parameters are given in Table 3.3. The specimens were preserved immediately after the loading regime by introducing a low viscosity, slow curing and low shrinkage epoxy resin PX672H (Robnor, 2012) via a gravity fed tube passing through the top platen and porous disc.

An additional triaxial test specimen was prepared according to established procedure but not tested. Instead, it was impregnated with resin after the specimen preparation steps were completed (Figure 3.6 right). This ‘Unloaded’ specimen is then used to study the fabric that develops as a result of the specimen preparation method and the systematic artificial compaction used. It also provides a benchmark with which the sheared specimens are compared.
Table 3.1 Information on the large scale specimens revived from the field and laboratory.

<table>
<thead>
<tr>
<th>Specimen</th>
<th>Location</th>
<th>Mineralogy</th>
<th>Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Arundel (ARU)</td>
<td>Arundel station</td>
<td>Limestone</td>
<td>End of life</td>
</tr>
<tr>
<td>New Milton (NWM)</td>
<td>1.25 km West of New Milton station</td>
<td>Limestone</td>
<td>End of life</td>
</tr>
<tr>
<td>Camberly (CAM)</td>
<td>1.56 km East of Camberly station</td>
<td>Limestone/Flint</td>
<td>End of life</td>
</tr>
<tr>
<td>High Marnham (HMA)</td>
<td>NR test track</td>
<td>Granitoid</td>
<td>2-3 years</td>
</tr>
<tr>
<td>LRig</td>
<td>Lab axel load sim.</td>
<td>Granitoid</td>
<td>-</td>
</tr>
<tr>
<td>Loose</td>
<td>Lab</td>
<td>Granitoid</td>
<td>-</td>
</tr>
</tbody>
</table>

Figure 3.6 Resin preserved specimens taken from a triaxial cell apparatus. (Left) Tested specimen. (Right) Unloaded specimen

Table 3.2 Initial void ratio and bulk density of triaxial test specimens (Aingaran 2014)

<table>
<thead>
<tr>
<th>Name</th>
<th>Initial bulk density $\rho_i$ (kg/m$^3$)</th>
<th>Initial $e_{ini}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unloaded</td>
<td>-</td>
<td>0.710</td>
</tr>
<tr>
<td>T1</td>
<td>1549</td>
<td>0.712</td>
</tr>
<tr>
<td>T2</td>
<td>1550</td>
<td>0.709</td>
</tr>
<tr>
<td>T3</td>
<td>1536</td>
<td>0.725</td>
</tr>
</tbody>
</table>
Table 3.3 Loading history for the triaxial test specimens (after Aingaran 2014)

<table>
<thead>
<tr>
<th>Name</th>
<th>Test stage</th>
<th>Deviator stress $q$ (kPa)</th>
<th>Confining stress $\sigma_3$ (kPa)</th>
<th>Maj principal stress $\sigma_1$ (kPa)</th>
<th>No. cycles</th>
<th>Max axial disp. (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>T1</td>
<td>Cyclic</td>
<td>5 - 225</td>
<td>15 - 45</td>
<td>--</td>
<td>1000</td>
<td>+10.20</td>
</tr>
<tr>
<td>T2</td>
<td>Cyclic</td>
<td>5 - 225</td>
<td>15 - 45</td>
<td>--</td>
<td>1000</td>
<td>+15.25</td>
</tr>
<tr>
<td></td>
<td>Extension</td>
<td>5 – (-150)</td>
<td>45 - 200</td>
<td>50</td>
<td>--</td>
<td>-8.10</td>
</tr>
<tr>
<td>T3</td>
<td>Cyclic</td>
<td>5 - 225</td>
<td>55</td>
<td>--</td>
<td>1000</td>
<td>+9.20</td>
</tr>
<tr>
<td></td>
<td>Extension</td>
<td>5 – (-150)</td>
<td>55 - 210</td>
<td>60</td>
<td>--</td>
<td>-2.00</td>
</tr>
<tr>
<td></td>
<td>Cyclic</td>
<td>5 - 225</td>
<td>55</td>
<td>--</td>
<td>1600</td>
<td>+9.20</td>
</tr>
</tbody>
</table>

Figure 3.7 Intended stress paths taken by triaxial tests mentioned in Table 3.3.
3.3. X-ray computed tomography of ballast bed specimens

X-ray Computed Tomography (XCT) provides a means for non-destructive observation and analysis of internal volumes. It is based, as with conventional radiography, on the attenuation of X-rays following interaction with matter and subsequent tomographic reconstruction of a series of 2D projections (or radiographs) taken from a range of angles (Figure 3.8). A brief overview of the fundamental concepts associated with X-ray and CT can be found in the appendix.

3.3.1. Scanning

The XCT scanner used in this project was a Nikon/Metris custom design machine built around a 450W (450kV, 1000μA) X-ray source combined with a flat panel or area detector (2000×2000 pixels) and a Curvilinear detector array (CLDA, 1024 pixels). The maximum spatial resolution ranges from 3 μm below 150 kV to 50 μm at 450kV. Due to the highly attenuating nature of hard rock such as granite, a combination of the CLDA and a collimated fan beam was used. The specimen setup and the CT system used in the imaging is shown in Figure 3.9.

3.3.2. Image quality

Image quality in CT tends to be relative to the specimen being scanned and the quantitative/qualitative requirement of the experiment. Image quality is usually measured in terms of contrast and spatial resolution or definition.

The contrast between different parts of the image is what forms the image and the greater the contrast, the more visible features become. It is primarily dependent on the absorption differences (attenuation coefficient) in the components of the specimen. Image contrast tends to degrade as the power W (i.e. a given combination of voltage and current) is increased (Crouse et al. 2014). Generally there is a trade-off between image contrast and specimen size/density. As the specimens gets denser/larger (or both), the power needs to be raised to enable penetration. Consequently, contrast between phases/materials suffers (Figure 3.10). The density of the ballast material and the overall diameter of the retrieved specimens necessitated the use of powers in excess of 220W in all cases.
And since the preserved ballast specimens consist of material phases (air, resin and granite) that are sufficiently different in density, the contrast between the phases was within acceptable limits.

The maximum achievable spatial resolution (for the equipment setup) is a function of the magnification (source-to-detector distance and the specimen-to-detector distance) and the focal spot size. Resolution reduces as the magnification reduces i.e. zooming out is required to fit the specimen in the available field of view. Spatial definition also reduces as the power is increased to penetrate dense specimens. This is a consequence of systematic defocusing of the source focal-spot on the target (anode) with increasing power which causes an edge blurring artefact called the penumbra (Figure 3.11). The defocusing helps minimise damage to the target when the power output is at the high end of the scale as is the case here. Even so, the minimum spatial resolution of 0.35 mm that has been achieved is fit for purpose since the smallest feature of interest is in the region of 6mm (corresponding to the smallest particle size in in the 1/3 scale lab specimens).

3.3.3. **Image acquisition**

There are two main parameters that control image recording; exposure time per frame and number of projections. The exposure time dictates how long the detector is allowed to collect X-ray photons to form the image. In general increasing the exposure time and reducing power will tend to improve the image quality of large and/or dense specimens. However, this is not economical as beam time is costly. So, higher power was used to reduce the exposure time as much as possible while making sure that the image quality was usable.

The preferred number of angular projections is as a rule of thumb, $\frac{\pi}{2} N_{pix}$, where $N_{pix}$ is the number of pixels along the width of the detector. However this can be optimised depending on the specimen and the feature of interest (Figure 3.12). Table 3.4 and Table 3.5 presents the final parameter settings used for the large scale and triaxial test specimens respectively.
Figure 3.8 Schematic of the principle of CT scanning and reconstruction, showing the experimental set-up (top) and corresponding reconstructed slice view (bottom). (ASTM International 2005)

Figure 3.9 Nikon-Metris custom designed industrial CT scanner
Figure 3.10 A comparison of image quality (Crouse et al. 2014).

Figure 3.11 Blurring or penumbra artefact induced by focal-spot defocusing (Crouse et al. 2014).
Figure 3.12 Illustration of filtered back projection for various numbers of angular projections

Table 3.4 µCT scan information for Large scale specimens

<table>
<thead>
<tr>
<th></th>
<th>Resolution (mm)</th>
<th>Voltage (kV)</th>
<th>Current (µA)</th>
<th>Power (Watts)</th>
<th>Exposure (ms)</th>
<th>No. Projections</th>
<th>Duration (hrs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ARU</td>
<td>0.3074</td>
<td>400</td>
<td>581</td>
<td>232.4</td>
<td>160</td>
<td>1201</td>
<td>24.02</td>
</tr>
<tr>
<td>NWM</td>
<td>0.2899</td>
<td>440</td>
<td>525</td>
<td>231.0</td>
<td>180</td>
<td>1201</td>
<td>51.76</td>
</tr>
<tr>
<td>CAM</td>
<td>0.3763</td>
<td>420</td>
<td>600</td>
<td>252.0</td>
<td>80</td>
<td>721</td>
<td>6.01</td>
</tr>
<tr>
<td>LJRig</td>
<td>0.2678</td>
<td>430</td>
<td>525</td>
<td>225.8</td>
<td>100</td>
<td>2001</td>
<td>65.59</td>
</tr>
<tr>
<td>HMA</td>
<td>0.3073</td>
<td>400</td>
<td>581</td>
<td>232.4</td>
<td>160</td>
<td>1201</td>
<td>24.02</td>
</tr>
<tr>
<td>Loose</td>
<td>0.3529</td>
<td>440</td>
<td>805</td>
<td>354.2</td>
<td>350</td>
<td>300</td>
<td>12.02</td>
</tr>
</tbody>
</table>

Table 3.5 Scan information for Triaxial apparatus specimens

<table>
<thead>
<tr>
<th></th>
<th>Resolution (mm)</th>
<th>Voltage (kV)</th>
<th>Current (µA)</th>
<th>Power (Watts)</th>
<th>Exposure (ms)</th>
<th>No. Projections</th>
<th>Duration (hrs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unloaded</td>
<td>0.2403</td>
<td>420</td>
<td>600</td>
<td>252</td>
<td>80</td>
<td>721</td>
<td>21.82</td>
</tr>
<tr>
<td>T3</td>
<td>0.2403</td>
<td>420</td>
<td>600</td>
<td>252</td>
<td>80</td>
<td>721</td>
<td>19.56</td>
</tr>
<tr>
<td>T1</td>
<td>0.2403</td>
<td>420</td>
<td>600</td>
<td>252</td>
<td>80</td>
<td>721</td>
<td>20.24</td>
</tr>
<tr>
<td>T2</td>
<td>0.2403</td>
<td>420</td>
<td>600</td>
<td>252</td>
<td>80</td>
<td>721</td>
<td>20.72</td>
</tr>
</tbody>
</table>
3.3.4. Image reconstruction

There are a number of methods by which the X-ray attenuation data can be converted into an image, some proprietary. The most commonly used approach is called filtered backprojection, in which the linear data acquired at each angular orientation are convolved with a specially designed filter and then backprojected across a pixel field at the same angle. The theory of reconstruction of two-dimensional functions from their projections is highly complex and is outside the scope of this thesis. A detailed treatment on this can be found in the books of Kak and Slaney (1987) and Natterer (1986) among others.

Reconstructed XCT data is predominantly stored and presented as a 3D matrix of image elements known as ‘voxels’, analogous to pixels in 2D images, but with a cuboidal geometry (Figure 3.13). Spatial resolution in XCT is reported in voxels.

![Diagram](image)

Figure 3.13 (A) 2D images are composed of discrete units of area called pixels. (B) 3D image datasets are composed of units of volume called voxels. (C) Voxels are usually \( x=y=z \)

3.3.5. Image post processing

Prior to quantitative analysis, the volume must be segmented into its constitutive phases (e.g. ballast, resin and air). Also, contacting particles forming clumps need to be separated into discrete volumes. In certain cases, artefacts such as image noise and variations in grayscale need to be minimized through filtration before segmentation and separation can be carried out.

In this section, a brief description is given of the filtration and segmentation/separation methodology used.
**Noise Filtering**

Figure 3.14 shows horizontal slices taken from two different specimens. The top image, taken from the SRTF, has no discernible noise making segmentation straightforward. The bottom image taken from the Arundel specimen, on the other hand, is sufficiently noisy to hinder acceptable segmentation and some form of noise reduction algorithm needs to be applied. Amongst the various noise filtering methods available, median based algorithms are best suited to applications where the preservation of edges or boundaries between different phases is important as in this case. A description of a standard median filtering algorithm in 2D is given in Section 4.2.2. The extension of the algorithm to 3D is trivial but the kernel size triples adding to computational cost. Figure 3.15 shows the effectiveness of median filtering in removing noise without merging separate particles.

**Segmentation and particle separation**

Image segmentation is the process of dividing an image into different parts. This is typically used to identify region/s of interest in digital images. The simplest segmentation method for CT data is intensity histogram based thresholding that uses the intensity value of the voxels as a means of identifying the phase or material it belongs to.

An intensity histogram is a graph showing the number of voxels in an image at each different intensity value found in that image. For the images considered in this study there are three main phases, the ballast phase, the resin phase and the air void phase. The intensity or brightness of each voxel is directly related with the density of the phase it represents. Figure 3.16 shows how the histogram profile changes as a line passes through the three different phases.

Depending on the number of different types of materials that are present in a specimen, histograms can be bi-modal or multi-modal. The key parameter in the thresholding process is the choice of the threshold value; some approaches use more than one threshold value (e.g., Oh and Lindquist, 1999). Different methods exist for finding the threshold value. A simple approach might be to use the lowest point in the valley of the histogram. However, even after filtering, finding the
minimum between the two peaks can be difficult. Threshold values can also be selected based on statistics such as the mean grey value (or range) of the phase of interest. However, this approach is complicated by the finite resolution of the imagery.

Because each data voxel encompasses a volume of material, if more than one material is present in that volume, the resulting CT grayscale will be some average of the phases present; this is known as the partial volume effect (PVE). Furthermore, some blurring is inevitable, causing the grayscale value within a voxel to be influenced by surrounding material. Thus material boundaries, rather than being sharp, will often extend across 2–4 voxel widths featuring a gradual grayscale transition between the end-member values characterizing each phase (Ketcham 2005).

Consequently, a trainable segmentation approach, implemented in the open source image processing package Fiji (Schindelin et al., 2012), was used. Kayning et al. (2010) developed the technique for the classification of neurons in serial-section transmission electron-microscopy (ssTEM) data. The approach allows the user to classify regions of pixels belonging to a number of distinct material classes (air, resin, ballast) within a single slice of the RAW grey-level CT data, and uses a random forest method, following Breiman (2001), for classification of voxels in the entire dataset. The algorithm uses a combination of well-defined image filters (i.e. the difference between two Gaussians, the local gradient given by Sobel filtering and the computation of $2\times2$ Hessian matrices) to define a range of descriptive parameters for each image pixel. The user trains the random forest classifier by manually defining specimen sets of voxels for each material class. The statistical method of bootstrapping (sampling with replacement) is used to parameterise the classifier, using the descriptive parameters of each user-defined pixel set to establish conditions determining the class to which a given test voxel is most likely to belong. The random forest algorithm is then applied to the entire dataset, allocating every voxel to the most probable parent class.
Figure 3.14 Horizontal slice through the lab sleeper rig (top) and Arundel specimen (bottom).
Figure 3.15 Noise reduction using 3D media filtering. (Left) Raw image. (Right) Filtered image

Figure 3.16 Grayscale profile of a line (yellow) through a slice
Figure 3.17 Semi-transparent overlay of selection made using a grayscale range (in red) and trainable segmentation (in green) from two locations.

Figure 3.17 compares segmentation based on the thresholding average maximum/minimum range of the ballast phase and the trainable segmentation algorithm. The images are a composite of the grayscale image overlain with a colorized mask of the segmented image. The segmentation done using thresholding (in red) tends to have holes in its selection of voxels. This is caused by the presence of higher than average density minerals in the rock. The TSA can be taught to include these brighter minerals. Additionally, a halo of sorts can be seen around each of the segmented regions when thresholding is used. This is a consequence of the PVE described above and will result in underestimation of a particle’s volume, surface area and to a lesser extent its major and minor diameters. The TSA handles this by implementing the sobel edge detection algorithm to define the boundary between two phases resulting in a better segmentation.

Following segmentation, contacting particles are separated using a high-level combination of the fast watershed, distance and numerical reconstruction algorithms found in the [off-the-shelf] volume analysis application Avizo Fire 7.1 (FEI, Oregon USA) which allows the process to be automated. The separation
can be done manually; however, specimens have hundreds and thousands of particles with contacts numbering an order of magnitude higher, making this impractical. An example of automated separation is shown in Figure 3.18. The voxels removed to separate connected particles are considered to represent the contact patch between them (e.g. Figure 3.19 and Figure 3.20). Ultimately, there are situations where computer vision either fails to separate connected particles (Figure 3.21 and Figure 3.22) or incorrectly splits a particle into two (Figure 3.23 and Figure 3.24). These errors have a direct and inverse relationship with the quality of the initial data acquisition (or scan). In the worst case scenario, in this instance the Arundel specimen, it was found that only 14 (or 1.79%) out of 780 particles failed to be separated and only 30 particles (or 3.85%) were incorrectly split into two or more fragments. On the other hand, specimens that were unaffected by imaging artefacts (e.g. LRig) had a combined (incorrect split plus un-separated) error of less than 1%. Once identified, these particles are repaired and replaced into the dataset. This means near 100% accuracy is achieved in terms of particle separation.

All the large scale specimens were physically reshaped to an octagonal prism using a diamond saw before scanning. This means that almost all the particles on the boundary have been cut through and are thus unrepresentative in shape and size of the rest of the specimen. While there are algorithms that are able to identify and remove boundary particles from 3D datasets, they only work on the external boundaries of a square/rectangular image. As a result, special algorithms were developed that allowed automatic identification and removal of objects associated with a polygonal boundary inside a square/rectangular image. Once identified, the boundary particles are subtracted from the original dataset leaving only the internal particles. This can be seen in Figure 3.25.
3. Analysis of fabric in railway ballast

Figure 3.18 Left: Before separation of particles. Right: After separation.

Figure 3.19 Voxels removed during the particle separation process shown in Figure 3.18.

Figure 3.20 Three dimensional rendering of contact patches
Figure 3.21 Particle not disconnected by automatic separation algorithm

Figure 3.22 3D rendering of conjoined particle

Figure 3.23 Splitting of one particle by automatic separation algorithm
3. Analysis of fabric in railway ballast

Figure 3.24 3D rendering of a particle split into two parts.

Figure 3.25 3D render of boundary particle in orange and internal particle in grey. The boundary particle are eliminated for prior to analysis.
3.3.6. Volume analysis

*Void ratio.*

The densitometric information available from a CT scan can provide an accurate measure of specimen void ratio that is free of boundary effects and unaffected by inaccurate measurement of the grain specific gravity or density of the material.

Analysis is carried out on a representative internal volume cropped out of the original dataset. Figure 3.26 shows how a virtual cylinder is used to extract a core from within the boundaries of the original specimen. The total volume of the cylinder in calculated as the sum of all voxels occupied by all the material phases i.e. air, resin, ballast (Figure 3.27 left). The volume of solids is calculated as before but only for the ballast material. (Figure 3.27 right).

The void ratio $e_{ct}$ is then

$$e_{ct} = \frac{V_v}{V_s}$$

(3.7)

where $V_s$ is the volume of solids and $V_v$ is the volume of voids and is calculated as the total volume minus the volume of solids.

*Particle orientation and dimensions.*

Particle orientation is measured in degrees on a spherical coordinate system and described by two angles that pertain to the indination of the object’s major and minor axes to a reference axis (Oda, 1972a).

Figure 3.28 shows the convention adopted here. The inclination or zenith angles for the major axis $\psi_{maj}$ and minor axis $\psi_{min}$ are measured from the horizontal axis and range between $0^\circ$ and $180^\circ$ where $90^\circ$ is vertical.
Figure 3.26 Taking a region of interest using a cylinder

Figure 3.27 Left: 3D volume of resin and ballast. Right: rendering of ballast particles only
For completeness, the azimuth angles for the major $\theta_{maj}$ and minor axis $\theta_{min}$ are measured from the horizontal reference axis (e.g. [1, 0, 0]) and range between $0^\circ$ and $180^\circ$. Determining the orientation of an object in 3D is simplest and perhaps most efficient when the orientation is defined as the direction of its major axis of inertia. While this works well with simple and roughly convex objects, it tends to be unreliable with railway ballast where the form of the particles can differ greatly from a convex shape. The alternative used here associates the orientation of the particle with the orientation of the maximum caliper/Feret diameter or major axis of the particle.

The caliper diameters of a three dimensional object can be measured by bounding the particle, represented as a set of discrete points that make up the surface (Figure 3.29), in a rectangular prism where the longest and shortest (non-diagonal) dimensions of the box correspond to the length and width of the object. However, measurements made using bounding box algorithms are prone to variations with rotational transformation (Section 4.2.3). To overcome this limitation, the bounding box is rotated at $1^\circ$ intervals, about the particle centre, in the $\theta$ and $\psi$ directions as shown in Figure 3.30. The orientation of the particle then corresponds to the $\theta$ and $\psi$ angle at which the longest dimension is measured. This method also allows the measurement of a secondary orientation in terms of the smallest diameter or minor axis of the particle. In this case the $\theta$ and $\psi$ angles
at which the smallest diameter occurs are used. It should be noted that the measured minor axis is not necessarily orthogonal to the major axis. The Bounding box algorithms implemented in Avizo Fire tends to become increasingly expensive computationally as the rotation interval gets finer. This is shown in Figure 3.31. At a rotational interval of 1°, 32400 unique bounding boxes are fitted to the particle. Computational cost can be reduced significantly through optimization. As a first step, the number of surface points is reduced through the use of a convex hull where the particle is tightly wrapped with a surface mesh (Figure 3.32A) and the points that intersect the surface of the hull are kept (Figure 3.32B and C). This filtering method reduces the number of points the bounding box algorithm has to scan through by 86% on average without losing any dimensional information on the particle. In addition to this, the discrete nature of the individual particles means that the execution of bounding box algorithms on each particle can be parallelized with further efficiencies gained through simultaneous multithreading.

The orientation of the particle's major axis can also be determined by fitting a circumscribed sphere as shown in Figure 3.33. This method is highly efficient, especially when used in conjunction with the convex hull point filtering mentioned above. However, bounding sphere algorithms are unable to measure the minor axis of the particle yielding incomplete dimension and orientation information about the particle.
3. Analysis of fabric in railway ballast

Figure 3.29 Cloud of points that make up the surface of a particle

Figure 3.30 Degrees of freedom for a bounding box encompassing a particle
Figure 3.31 relation between rotational precision of the bounding box and the associated number of iteration.

Figure 3.32 reducing the number of surface points using a convex hull. 
A: convex hull (transparent red) encompassing the particle, B: red points are where the convex hull and the particle touch and C: the points that are used in the bounding box analysis.
Figure 3.33 Sphere Circumscribing a particle in order to measure its longest dimension.

Contact normal orientation and coordination number
The orientation of the contact normal is reported using the same convention described previously for particle orientation.

Contacts between crushed natural rocks such as railway ballast occur over a surface area at the macroscopic level. These ‘contact patches’ have irregular surfaces as shown in Figure 3.34. Consequently, a linear least squares regression algorithm was written in Matlab (MathWorks, Cambridge U.K.) to identify a plane of best-fit for the contact patch and the normal vector $V_n$ associated with the fitted plane is used to describe the orientation of the contact (Appendix D.2.). Computational efficiency is improved by using only the surface points of the contact patch. The algorithm works by minimizing the orthogonal distance from the points to the fitted plane as shown in Figure 3.35 and Figure 3.36.

The inclination angle $\psi_c$ of the normal vector of the fitted plane is simply the angle between its unit normal vector $U_n$ and the vertical standard basis $e_z$ or $[0, 0, 1]$ in Cartesian coordinates such that,
\[
\psi_c = \cos^{-1} U_n \cdot e_z
\]  

(3.8)

The azimuth angle \( \theta_c \) on the other hand is measured from the projection of \( U_n \) on to the horizontal plane described by \( e_x = [1, 0, 0] \) and \( e_y = [0, 1, 0] \) (Figure 3.28).

The average contact coordination number \( CN \) is calculated using Equation 2.6.

Figure 3.34 Isosurface rendering of a contact path. The yellow dots are the nodes of the surface mesh.
Figure 3.35 Plane fitted to the contact shown in Figure 3.40. The red line represents the normal vector of the fitted plane.

Figure 3.36 ZY view of the plane fitted to the contact seen in Figure 3.34. The green and blue lines represent the orthogonal distance from the surface of the contact patch to the fitted plane.
Figure 3.37 3D volume render of the particle pair associated with the contact patch in Figure 3.34 and the fitted plane.
3.4. Results

3.4.1. Triaxial test specimen

A total of four triaxial specimens were imaged using XCT. The state of the specimens and the scan parameters can be found in Section 3.13 and 3.32 respectively. Figure 3.38 presents the middle slice, in elevation view, of all specimens.

Void ratio

Table 3.6 shows the void ratio measurements from the laboratory $e_{lab}$ and the XCT data $e_c$. The $e_{lab}$ were back calculated from diameter measurements from local radial displacement transducers (Hall Effect type) and the final height of the specimens. The calculations were carried out on the assumption that the specimens were right circular cylinders. This is reasonable since no pronounced barrelling or shear band localisation was seen in any of the specimens tested (Figure 3.38). The end-of-test void ratio can also be calculated using the volume measurements recorded from the pressure controller. However, all the tests had significant membrane creep/penetration making volume measurements unreliable (Aingaran, 2014).

Experimental measurements of void ratio are larger than $e_{cT}$ in all four cases. This is because $e_{lab}$ is global and is unable to capture the variation of voids within the specimens. On the other hand, the void ratio obtained by voxel counting is far more precise since local variations are accounted for and boundary effects can be avoided by sampling an inner core. Even so, image based methods can be very sensitive to the threshold value selected during the image binarization process and also to errors associated with the finite voxel size. The average difference between the two methods of reporting $e$ is 12% and the maximum difference observed is 15% associated with T2 (Table 3.6).

CT data provide a unique opportunity to investigate the localised variation of voids within a specimen. Local measurements are carried out by virtually sectioning a specimen along the height or width (Figure 3.39) into a number of sections and then calculating the void ratio per section as before.
Figure 3.38 Vertical slice through (a) Unloaded (b) T1-cyclic (c) T2 - cyclic+extension and (d) T3 - cyclic +extension+cyclic
Table 3.6 End-of-test void ratios for all triaxial test specimens measured over whole sample. (Unloaded – unsheared, T1 – cyclic only, T2 – cyclic+extension and T3 – cyclic+extension+cyclic)

<table>
<thead>
<tr>
<th></th>
<th>Initial void ratio</th>
<th>End-of-test void ratio $e_{\text{tab}}$</th>
<th>End-of-test void ratio $e_{\text{ct}}$</th>
<th>Difference $(e_{\text{tab}}-e_{\text{ct}})/e_{\text{ct}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unloaded</td>
<td>0.710</td>
<td>0.710</td>
<td>0.616</td>
<td>15%</td>
</tr>
<tr>
<td>T1</td>
<td>0.712</td>
<td>0.645</td>
<td>0.582</td>
<td>10%</td>
</tr>
<tr>
<td>T2</td>
<td>0.709</td>
<td>0.656</td>
<td>0.570</td>
<td>15%</td>
</tr>
<tr>
<td>T3</td>
<td>0.725</td>
<td>0.638</td>
<td>0.587</td>
<td>8%</td>
</tr>
</tbody>
</table>

Figure 3.39 Illustration of virtual horizontal and vertical sectioning

Figure 3.40 shows the variation of void ratio over the specimen height. The horizontal sectioning was performed at 13.5 mm ($D_{50}$) intervals. The void ratio profile for the unloaded specimen is unusual in that the top half is uncharacteristically more porous than the rest of the specimen. It is not uncommon to have density variations in prepared specimens, especially when prepared by sequential compaction as is the case here. However, the magnitude of the variation suggests that the specimen is atypical and is possibly caused by over vibration resulting in segregation of the smaller particles to the lower layer of the specimen. A comparison of T1 and T2 indicates that extension has led to a lower void ratio in this case (Figure 3.40 and Table 3.6). Measurement of void ratio carried out by virtual vertical section also shows that extension in this case has actually reduced the void ratio in T2 (Figure 3.41). Although this seems counter-intuitive it can be explained by taking into consideration the initial void ratio (Table 3.6) and the loading conditions (Table 3.3). T2 started off at a lower
initial void ratio and was also axially strained (or shortened) by 50% more than T1 (Table 3.3). During extension only half of this strain was recovered. Consequently, the lower void ratio of T2 is plausible. In retrospect, the differences in final specimen height between T1 and T2 make void ratio comparison problematic.

T3 on the other hand exhibits behaviour similar to that of the unloaded specimen but less pronounced. Figure 3.41 presents the variation of void ratio along the specimen width. Vertical sectioning was performed at 13.5 mm ($D_{50}$) intervals. The void ratio profile of all the specimens along this direction is very similar and none exhibit any deviation from the norm. The previous anomalies seen in the unloaded and T3 specimen are no longer picked up because vertical sections cut through the entire height of the specimen (Figure 3.39) thus averaging out any local anisotropy that may be present as a result of the preparation method.

Figure 3.42 visualises the particle centroid locations and size information (circle size proportional to the major diameter and colour denoting particle volume). The region highlighted by the dashed line in the unloaded specimen is largely occupied by particles with volume $<2.5 \times 10^{-6}$ m$^3$. While immediately above and to the right there is a cluster of large particles. These local variations could be responsible for the aforementioned void ratio irregularity seen in the unloaded specimen (Figure 3.43). T1 appears to have a much larger proportion of particles in the volume range of $2 - 4 \times 10^{-6}$ m$^3$ which are almost uniformly distributed throughout the specimen. Overall, Figure 3.40 and Figure 3.41 show that experimental global measures of soil state indicator (e.g., void ratio) can be grossly misleading with regard to the quality of prepared specimens of ballast. It is not practical or economic to CT every specimen prior to testing and so greater care must be taken when preparing gravel sized granular media for triaxial testing since their roughness and angularity could induce inhomogeneity.

**Contact coordination number**

The average contact coordination number $CN$ for the unloaded, T1 T2 and T3 specimens is 6.78, 7.84, 8.48 and 8.39 respectively. The cyclic loading undergone by T1 equates to an increase of one (1.06) additional contact per particle
compared to the unloaded specimen. Stress reversal in compacted granular media rearranges the particles to resist the current load path. In the case of T2, the particle matrix is initially vertically compressed; the extension that follows was accompanied by a net increase of 50 kPa in the confining pressure. It is this higher pressure that causes the particle contacts to rearrange in the horizontal direction. The pre-existing fabric in the specimen had been configured to resist vertical loading; however when the principal stress is rotated by 90°, the particles are not able to reconfigure to their most efficient spatial arrangement due to the confinement. It is inferred that the higher $CN$ is needed to compensate for this. Others have also observed similar behaviour through numerical simulation using DEM, where a load reversal results in an increase in $CN$ (e.g., O’Sullivan & Cui 2009). Figure 3.43 shows the spatial distribution of contact centroids over the specimen height. The bin size was set $2.25\times D_{50}$ so that it was sufficiently large to average out particle scale variations (Jiang et al. 2003). As expected, the higher void ratios at the top of the unloaded specimen are associated with fewer contacts. A comparison between T1 and T2 shows that the reversal of stress (or extension loading) generally increases the number of contacts with no localisation taking place. T3 on the other hand shows a region of high contact concentration near the top as well as a region of low contact concentration at the bottom.

Figure 3.44 shows the correlation of void ratio and $CN$. The observable trend indicates an inverse relationship with $CN$ increasing with decreasing void ratio. There have been attempts to formulate expressions that relate these parameters (e.g., Hasan & Alshibli 2010). However, void ratio and $CN$ for real materials are not independent of other factors such as particle shape and size. This makes it very difficult to justify any such relationship.
Figure 3.40 Variation of void ratio along the height of the specimen. 0 (zero) is at the bottom of specimen.

Figure 3.41 Variation of void ratio along the width of the specimens.
Figure 3.42 Distribution of particle centroids where the circle diameter is a function of the particle’s smallest diameter and the colourmap a function of the particle volume. (a) Unloaded, (b) T1, (c) T2 and (d) T3
Figure 3.43 Spatial distribution of contact centroids at $2.25 \times D_{50}$ height intervals

Figure 3.44 Correlation between void ratio and average contact coordination number
Particle orientation and fabric

Assessment of the general state of particle orientation in a specimen can be made with the help of a rose diagram of the major diameter inclination angle $\varphi_{maj}$ of the particles. The orientation data has been binned at 15° intervals.

Figure 3.45 shows the rose diagrams of the particle orientations for all the triaxial cell specimens. The unloaded specimen shows a greater concentration around the horizontal plane i.e. perpendicular to the direction of deposition. This is undoubtedly a consequence of the specimen preparation process where the granular mass is poured into the split mould and then compacted using vibration with an overburden. As a result, nearly 60% of the particles are oriented at or below an orientation of 30°. Cyclic vertical loading (T1) does not significantly change the preferential orientation of the particles and as with the initial specimen, the majority ($\approx 58\%$) of the particles remain inclined close to the horizontal plane (Figure 3.45B). There is however a small but noteworthy increase in the number of particles oriented at 30-60° as a result of the cyclic loading reducing the number of near vertical particles. On the other hand, when a stress reversal is induced (T2), it causes a significant variation in the orientations of the
particles from the initial state. The number of particles oriented at or less than 15° reduces, with particle orientations being redistributed to between 15° and 45° (Figure 3.45C). There is also a slight increase in the number of particles oriented at or above 60°. This suggests that a principal stress rotation of 90° will have a measurable effect on the fabric of a granular material by inducing changes in the particle topology through rearrangement. Figure 3.45D shows the effects of cyclic vertical loading, following a rotation of the principal stress (T3). It is interesting to note that there are 5% fewer particles oriented between 30° - 60° and 2.50% more particles oriented between 60° - 90° in T3 than in T1.

For specimens such as these, the frequency distribution of the ψ angles for a specimen gives an indication of the fabric anisotropy. This distribution is determined by considering all the unit vectors describing the orientations to originate at the centre of a unit sphere. Then the number of vectors that intercept the surface of the sphere over an angular increment of Δψ (Figure 3.46) are counted and normalised by the total number of vectors. For an isotropic material the frequency distribution is determined by considering the incremental area ΔA associated with the angle increment (e.g. the hatched area in Figure 3.46) divided by the total surface area of the hemisphere. The resultant distribution takes the non-linear form illustrated in Figure 3.47 (ISO). This is because ΔA associated with ψ tending towards 90° (i.e. the apex or pole) is much smaller than ΔA value when ψ is approaching 0°. Owing to the finite numbers of particles in all the specimens, a degree of scatter will be seen in the results in Figure 3.47. The data presented in Figure 3.47 confirms trends seen in the rose diagrams. In comparison to an isotropic material, the triaxial cell specimens have far more particles oriented at 30° or less. All the specimens exhibit a peak in the distribution at or near 12.5°.

Figure 3.48 shows the spatial distribution of particles in term of their size (major diameter) and orientation (ψmaj). Overall it can be seen that particles that tend to be more vertical are also smaller in size.

The fabric tensor for the particle orientation was calculated using a Matlab script (see Appendix D.3) that implemented Equation 2.10. The 3D anisotropy or
deviatoric fabric was calculated using the methods described by Thornton (2000) in which the difference between the principal and minor eigenvalues of the fabric tensor is calculated, i.e. \( \lambda = \lambda_1 - \lambda_3 \). The values obtained of the deviator fabric are plotted in Figure 3.49. It shows that the intensity of anisotropy decreases with cyclic loading. This is counterintuitive as anisotropy is expected to increase with loading. It can be reasoned that cyclic loading destroys the inherent anisotropy leading to the formation a new but weaker induced anisotropy. This has been shown to happen in sand by Oda (1972a). Reversal of the stress path further degrades the induced anisotropy. Cyclic loading, after the load reversal, is not only unable to reverse the loss in anisotropy but actually helps to reduce it further. Given that the decrease in anisotropy is accompanied by an increase in coordination number, it can be concluded that the additional contacts that develop during the load reversals tend to be horizontally inclined (i.e. the vertical component of the normal contact force vector is smaller than the horizontal component). This suggests that the load reversals do not cause an increase in the number of strong force chains in the system (e.g., O’Sullivan & Cui 2009).
3. Analysis of fabric in railway ballast

Figure 3.46 Definition of equal angle sphere distribution

Figure 3.47 Distribution of particle major axis orientation $\psi_{maj}$ at 5° intervals. Unloaded. T1 – cyclically loaded only. T2 - cyclically loading followed by extension. T3 – Cyclic, extension and cyclically loaded. ISO – Isotropic distribution.
Figure 3.48 Distribution particle centroid where the circle diameter is a function of the particles major axis and the colourmap a function of the particle orientation. (a) Unloaded, (b) T1, (c) T2 and (d) T3
Figure 3.49 Evolution of particle orientation anisotropy (deviator fabric or $\lambda_1 - \lambda_3$) due to different loading regimes

Contact orientation and fabric

The triaxial specimens were prepared by pouring a known mass of material into a split mould in 3 layers. Each layer was vibrated for 1 minute under self-weight followed by vibration for 1 minute with a 5 kg weight on top of it (Aingaran 2014). As such, intuition would suggest that majority of contact normal, for the unloaded (Initial) specimen, would be pointing vertically (i.e. 90° from the horizontal) to resist the loading caused by the overburden. However, the contrary is shown in Figure 3.50A. About 60% of the contact normals in the Initial unloaded specimen are oriented between 0° - 30° from the horizontal. Therefore, majority of the contact patches are oriented between 90° - 60° from the horizontal respectively. This is not unexpected given the irregular shape of the scaled ballast and the method of specimen preparation. The 5 kg surcharge does apply a vertical load during preparation. However, this is somewhat mitigated by the vibration applied
which shakes the particle and pack them in closer together. As a consequence, majority of the contacts occur laterally. This can be seen clearly in Figure 3.38 where the combination of particle angularity and their random orientation results in few near vertical contacts and therefore resulting in contact normals that are near horizontal.

A comparison of the initial specimen and T1 (Figure 3.50A and B) shows that vertical loading causes a reduction of 12.5% in the number of contacts normals that are oriented between 0° - 30°. Concurrently, contact normals between 30° - 60° and 60° - 90° increase by 4.9% and 7.6% respectively. As expected, extension after cyclic loading (i.e. T2 compared to T1) has the opposite effect. The number of contact normals between 30° - 90° decrease by 6.23% while there is an equal increase in the 0° - 30° interval. Cyclic loading after extension (i.e. T3 compared to T1) did not have the same effect as cyclic loading from an unloaded specimen. T3 has roughly 10% more contacts normals oriented between 0° - 30°, while in the 60° - 90° interval, there are 7% fewer contact normals. Similar observations are made in Figure 3.51 where a comparison of frequency distribution curve for the contact normal orientation \( \Psi_c \) with the isotropic case is presented.

The contact normal orientation data shows that the initial fabric created during specimen preparation is modified by the cyclic loading whereby contacts rotate to resist the vertical load. Subsequent stress rotation reverses this to a great extent thereby destroying the fabric that was developed through cyclic loading. Finally, cyclic loading after a stress rotation is only capable of partial recovery of the initial fabric. The fabric tensor analysis for the contact normals is presented in Table 3.7. The eigenvalues (\( \lambda_1, \lambda_2, \lambda_3 \)) show the lack of any strong directional preference. This is a reasonable finding since the particles are of arbitrary shape with many facets that are oriented randomly, therefore contacts are devoid of any directional dependency giving rise to an isotropic fabric.

The deviator fabric of the contact normal orientation is given in Table 3.8 and plotted in Figure 3.52. A comparison with the particle orientation deviator fabric shows that the contact orientation fabric has substantially lower intensity of anisotropy confirming the lack of a strong directional preference.
Figure 3.50 Rose diagrams of contact normal orientation ($\psi_c$) measured from horizontal. A: Initial – unloaded. B: T1 – cyclically loaded only. C: T2 - cyclically loading followed by extension. D: T3 – Cyclic, extension and cyclically loaded.

Figure 3.51 Distribution of contact normal orientation $\psi_c$ at 5° intervals.
3. Analysis of fabric in railway ballast

<table>
<thead>
<tr>
<th>Specimen</th>
<th>Fabric tensor</th>
<th>Eigenvalue</th>
<th>Eigenvector</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unloaded</td>
<td>0.314 0.003 -0.0167</td>
<td>λ₁ = 0.357</td>
<td>( \hat{v}_1 = \begin{pmatrix} -0.365 \ 0.036 \ 0.930 \end{pmatrix} )</td>
</tr>
<tr>
<td></td>
<td>0.003 0.335 0.002</td>
<td>λ₂ = 0.335</td>
<td>( \hat{v}_2 = \begin{pmatrix} 0.149 \ 0.988 \ 0.020 \end{pmatrix} )</td>
</tr>
<tr>
<td></td>
<td>-0.167 0.002 0.350</td>
<td>λ₃ = 0.307</td>
<td>( \hat{v}_3 = \begin{pmatrix} -0.918 \ 0.146 \ -0.366 \end{pmatrix} )</td>
</tr>
<tr>
<td>T1</td>
<td>0.295 -0.002 0.0009</td>
<td>λ₁ = 0.393</td>
<td>( \hat{v}_1 = \begin{pmatrix} 0.010 \ -0.033 \ 0.999 \end{pmatrix} )</td>
</tr>
<tr>
<td></td>
<td>-0.002 0.311 -0.002</td>
<td>λ₂ = 0.311</td>
<td>( \hat{v}_2 = \begin{pmatrix} -0.135 \ 0.990 \ 0.034 \end{pmatrix} )</td>
</tr>
<tr>
<td></td>
<td>0.0009 -0.002 0.3927</td>
<td>λ₃ = 0.295</td>
<td>( \hat{v}_3 = \begin{pmatrix} 0.990 \ -0.136 \ -0.05 \end{pmatrix} )</td>
</tr>
<tr>
<td>T2</td>
<td>0.300 -0.0001 -0.006</td>
<td>λ₁ = 0.390</td>
<td>( \hat{v}_1 = \begin{pmatrix} -0.071 \ -0.031 \ 0.997 \end{pmatrix} )</td>
</tr>
<tr>
<td></td>
<td>-0.0001 0.3110 -0.002</td>
<td>λ₂ = 0.310</td>
<td>( \hat{v}_2 = \begin{pmatrix} 0.038 \ -0.998 \ -0.029 \end{pmatrix} )</td>
</tr>
<tr>
<td></td>
<td>-0.006 -0.0002 0.389</td>
<td>λ₃ = 0.300</td>
<td>( \hat{v}_3 = \begin{pmatrix} 0.996 \ 0.036 \ 0.073 \end{pmatrix} )</td>
</tr>
<tr>
<td>T3</td>
<td>0.311 0.0008 0.002</td>
<td>λ₁ = 0.351</td>
<td>( \hat{v}_1 = \begin{pmatrix} 0.047 \ -0.265 \ 0.963 \end{pmatrix} )</td>
</tr>
<tr>
<td></td>
<td>0.0008 0.338 -0.003</td>
<td>λ₂ = 0.337</td>
<td>( \hat{v}_2 = \begin{pmatrix} 0.053 \ 0.963 \ 0.263 \end{pmatrix} )</td>
</tr>
<tr>
<td></td>
<td>0.002 -0.003 0.350</td>
<td>λ₃ = 0.311</td>
<td>( \hat{v}_3 = \begin{pmatrix} 0.997 \ -0.038 \ -0.060 \end{pmatrix} )</td>
</tr>
</tbody>
</table>
Table 3.8 Intensity of anisotropy for the contact normal orientation for triaxial test specimens.

<table>
<thead>
<tr>
<th>Specimen</th>
<th>$\lambda_1 - \lambda_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unloaded</td>
<td>0.0494</td>
</tr>
<tr>
<td>T1</td>
<td>0.0972</td>
</tr>
<tr>
<td>T2</td>
<td>0.0895</td>
</tr>
<tr>
<td>T3</td>
<td>0.0401</td>
</tr>
</tbody>
</table>

Figure 3.52 Evolution of contact normal orientation anisotropy due to different loading regimes using $\lambda_1 - \lambda_3$. 
3.4.2 Field specimens

It should be noted that the High Marnham specimen was contaminated with coal slag. This can be seen in Figure 3.53. These particles were virtually removed (by image manipulation) prior to analysis. This was done for two reasons; first, the highly porous slag particles tend to be aggressively split by the automatic separation algorithm (for example see Figure 3.22) and secondly, they are not used, as a rule, as track building material since their mechanical and shape characteristics are inferior to hard rock ballast.

Also, the Camberly specimen was not analysed owing to its small size (Figure 3.54); the number of particles that remained after clearing partial edge particles was not representative of a typical track bed that is ≈300 mm deep.

Figure 3.53 Left: Horizontal slice at top of HMA specimen. Right: at bottom of HMA specimen.

Figure 3.54 Vertical cross section from CAM
Void ratio

The void ratio $e_{cl}$ for each of the large scale specimens is given in Table 3.11. Figure 3.55 shows the void ratio at 40mm ($D_{50}$) intervals. The Loose specimen has the highest void ratio while ARU has the lowest closely followed by NWM. This similarity in void ratio between ARU and NWM is most likely due to the loading type and history. There is also the possibility that particle shape had an effect since both ARU and NWM have limestone ballast with potentially similar particle shapes resulting in similar compaction characteristics. The LRig is shown to have differential densification. Although the specimen was subjected to 1 million load cycles, the localised reduction in void ratio suggests that this could have been due in part to the finite size of the experimental setup (Figure 3.5).

Contact coordination number

The CN for each of the specimens is given in Table 3.9. In general, the measured CN for the large scale specimens are nominally larger by a third compared with the values reported for the triaxial specimens previously. CN for HMA is distinctly lower than other specimens because of the removal of coal slags (Figure 3.53) and the associated contacts from the analysis. The ballast in Loose and LRig specimens are from the same parent rock and therefore comparable while the ballast in the ARU and NWM specimen are both Limestone.

<table>
<thead>
<tr>
<th></th>
<th>Void ratio ($e_{cl}$)</th>
<th>CN</th>
</tr>
</thead>
<tbody>
<tr>
<td>Loose</td>
<td>0.8403</td>
<td>12.16</td>
</tr>
<tr>
<td>LRig</td>
<td>0.7093</td>
<td>13.93</td>
</tr>
<tr>
<td>NWM</td>
<td>0.6043</td>
<td>12.62</td>
</tr>
<tr>
<td>HMA</td>
<td>0.7307</td>
<td>3.61</td>
</tr>
<tr>
<td>ARU</td>
<td>0.5621</td>
<td>12.74</td>
</tr>
</tbody>
</table>

Table 3.9 Void ratio and CN for all large scale specimens
Figure 3.55 Variation of void ratio with specimen height at a horizontal slice thickness of 40mm

Figure 3.56 Rose diagrams of particle major axis ($\theta_{maj}$) orientation from horizontal. 
A: Loose. B: LRig. C: NWM. D: HMA E: ARU
Particle orientation and fabric

Figure 3.56 shows the rose diagrams of the orientation (from the horizontal) of the particle major axis $\psi_{maj}$ for all the large scale specimens. As with the triaxial specimens, all the specimens show a strong orientation preference of less than 30°. Furthermore, cyclic vertical loading (in the field and lab) does not change the preferred orientation significantly from the loose state (Figure 3.56A and B). The majority of the particles remain at an orientation of less than 30°, echoing the results seen with the triaxial specimens (i.e. Unloaded and T1).

Figure 3.57 compares the $\psi_{maj}$ data with the isotropic case. It shows that the Loose specimen lacks a distinct peak instead a gradual decrease is seen in the number of particles as orientation becomes steeper. This is because the Loose specimen did not undergo any vibration or normal loading prior to scanning. The LRig shows the effects of cyclic loading on large scale ballast. Its shows that the response to cyclic loading in 1/3 scaled ballast and full sized ballast are comparable. Both LRig and T1 have peak at 12.5° (i.e., midpoint of the 10° – 15° bin) and intersect the isotropic line at an orientation of $\approx 30°$. Like the triaxial test specimen, all the specimens in Figure 3.57 have at least a third of their particles oriented between 0 and 15°.

The intensity of anisotropy or deviator fabric is plotted in Figure 3.58. As previously seen (Figure 3.49), cyclic loading does indeed break up the inherent anisotropy (or initial fabric) and load induced anisotropy is not as pronounced.
3. Analysis of fabric in railway ballast

Figure 3.57 Distribution of particle major axis orientation $\psi_{maj}$ for large scale specimens at 5° intervals

Figure 3.58 Graphical comparison of the deviator fabric in the particle orientation of all large scale specimens
Contact orientation and fabric

Figure 3.59 shows the rose diagrams for the orientation of the contact normal for the large scale specimens. It can be seen from Figure 3.59A that more than 50% of contact normals are oriented at or less than 15°. This is due to the absence of any load history. Cyclic loading (LRig) initiates a process whereby contact normals oriented horizontally break and new contacts that are created orient themselves normal to the direction of loading. This can be seen in Figure 3.59B where the number of contacts oriented at or less than 15° reduces by 25% compared to the loose specimen and are evenly redistributed between 15°-90°.

This is also confirmed in Figure 3.60 where the graph for the L Rig specimen shows a sharp drop between 0 - 15° compared with the loose specimen followed by an almost equal distribution of contact normals between 15° and 90°. Similar observations may be made between the unloaded and T1 specimens. The contact normal distribution plots of NWM and ARU (Figure 3.60) resemble closely those of T2 and T3. This could suggest that specimens taken from Arundel and New Milton were subjected to some form of stress reversal (e.g. tamping) during their life.

The fabric tenor analyses for the large scale specimens are presented in Table 3.10 and Table 3.11. The deviator fabric for the contact normals is presented in Figure 3.61. It can be seen that cyclic loading increases the intensity of the anisotropy of the contact normals. This is consistent with what was observed with the traxial test specimens.
Figure 3.59 Rose diagrams of contact normal orientation ($\psi_c$) from horizontal. A: Loose. B: LRig. C: NWM. D: HMA E: ARU

Figure 3.60 Distribution of particle major axis orientation $\psi_c$ for large scale specimens.
### Table 3.10 Contact normal orientation fabric tensor analysis for large scale specimens.

<table>
<thead>
<tr>
<th>Specimen</th>
<th>Fabric tensor</th>
<th>Eigenvalue</th>
<th>Eigenvector</th>
</tr>
</thead>
</table>
| Loose    | \[
\begin{bmatrix}
0.366 & -0.011 & 0.004 \\
-0.011 & 0.384 & 0.006 \\
0.004 & 0.006 & 0.249
\end{bmatrix}
\] | \(\lambda_1 = 0.386\) | \(\hat{v}_1 = \begin{pmatrix}
-0.418 \\
0.907 \\
0.028
\end{pmatrix}\) |
|          | \(\lambda_2 = 0.361\) | \(\hat{v}_2 = \begin{pmatrix}
0.907 \\
0.415 \\
0.062
\end{pmatrix}\) |
|          | \(\lambda_3 = 0.248\) | \(\hat{v}_3 = \begin{pmatrix}
-0.044 \\
0.052 \\
0.997
\end{pmatrix}\) |
| LRig     | \[
\begin{bmatrix}
0.259 & -0.003 & -0.001 \\
-0.003 & 0.287 & -0.014 \\
-0.001 & -0.014 & 0.453
\end{bmatrix}
\] | \(\lambda_1 = 0.454\) | \(\hat{v}_1 = \begin{pmatrix}
-0.008 \\
-0.083 \\
0.996
\end{pmatrix}\) |
|          | \(\lambda_2 = 0.286\) | \(\hat{v}_2 = \begin{pmatrix}
-0.119 \\
0.989 \\
0.081
\end{pmatrix}\) |
|          | \(\lambda_3 = 0.258\) | \(\hat{v}_3 = \begin{pmatrix}
0.992 \\
0.118 \\
0.018
\end{pmatrix}\) |
| NWM      | \[
\begin{bmatrix}
0.357 & -0.008 & 0.004 \\
-0.008 & 0.379 & -0.031 \\
0.004 & -0.031 & 0.262
\end{bmatrix}
\] | \(\lambda_1 = 0.390\) | \(\hat{v}_1 = \begin{pmatrix}
0.274 \\
-0.931 \\
0.236
\end{pmatrix}\) |
|          | \(\lambda_2 = 0.355\) | \(\hat{v}_2 = \begin{pmatrix}
-0.961 \\
-0.272 \\
0.044
\end{pmatrix}\) |
|          | \(\lambda_3 = 0.2544\) | \(\hat{v}_3 = \begin{pmatrix}
-0.023 \\
0.240 \\
0.970
\end{pmatrix}\) |
| HMA      | \[
\begin{bmatrix}
0.383 & 0.044 & -0.077 \\
0.044 & 0.301 & 0.019 \\
-0.077 & 0.019 & 0.315
\end{bmatrix}
\] | \(\lambda_1 = 0.439\) | \(\hat{v}_1 = \begin{pmatrix}
-0.846 \\
-0.200 \\
0.493
\end{pmatrix}\) |
|          | \(\lambda_2 = 0.322\) | \(\hat{v}_2 = \begin{pmatrix}
0.142 \\
0.807 \\
0.572
\end{pmatrix}\) |
|          | \(\lambda_3 = 0.237\) | \(\hat{v}_3 = \begin{pmatrix}
0.513 \\
-0.554 \\
0.655
\end{pmatrix}\) |
| ARU      | \[
\begin{bmatrix}
0.372 & 0.003 & 0.018 \\
0.003 & 0.342 & -0.008 \\
0.018 & -0.008 & 0.285
\end{bmatrix}
\] | \(\lambda_1 = 0.376\) | \(\hat{v}_1 = \begin{pmatrix}
-0.980 \\
-0.045 \\
-0.192
\end{pmatrix}\) |
|          | \(\lambda_2 = 0.343\) | \(\hat{v}_2 = \begin{pmatrix}
-0.016 \\
0.988 \\
-0.149
\end{pmatrix}\) |
|          | \(\lambda_3 = 0.280\) | \(\hat{v}_3 = \begin{pmatrix}
-0.197 \\
0.143 \\
0.969
\end{pmatrix}\) |
Table 3.11 Intensity of anisotropy in contact normal orientation for large scale specimens

<table>
<thead>
<tr>
<th>Specimen</th>
<th>$\lambda_1 - \lambda_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Loose</td>
<td>0.141</td>
</tr>
<tr>
<td>LRight</td>
<td>0.196</td>
</tr>
<tr>
<td>NWM</td>
<td>0.136</td>
</tr>
<tr>
<td>HMA</td>
<td>0.202</td>
</tr>
<tr>
<td>ARU</td>
<td>0.096</td>
</tr>
</tbody>
</table>

Figure 3.61 graphical comparison of the deviator fabric in the contact normal orientation for large scale specimens.
3.5. Summary

This chapter has used a novel sampling technique that, for the first time, has allowed the extraction of specimens from rail track ballast beds with their fabric intact. It has been successfully implemented under field conditions in multiple locations with differing environmental/operational situations and has proved to be a robust, reliable and fast solution. Heavy fouling was not encountered at any of the sampling sites, and it is recognized that the resin sampling technique may be less suitable for locations where heavy fouling has occurred.

The novel use of X-ray CT technology has enabled non-destructive 3D imaging of granular media at an unprecedented scale and fidelity. This allowed the analysis of the internal fabric of ballasted rail tracks as it occurs in the field. Furthermore it was also shown that the fabric of large scale triaxial cell specimens can be analysed over the *whole* specimen. This is a step change since all previous X-ray imaging and analysis of laboratory soil elements test has been carried out on sands where only a small internal volume of the specimen was scanned and analysed (e.g., Fonseca *et al.* 2012; Oda *et al.* 2004) with the assumption that the findings hold true for the whole specimen.

Void ratio analysis of whole triaxial test specimens showed that the homogeneity within the specimen is difficult to judge using global experimental measures. The observations reinforce the need for careful and systematic specimen preparation techniques in situations where the granular material being handled is gravel sized angular particles capable of developing strong interlocked fabric. Alternatively, larger specimen size could also be used.

The findings indicate that cyclic loading will modify existing fabric through a combination of particle and contact normal reorientation. The fabric that subsequently develops (due to cyclic loading) is as a result of reduced particle anisotropy and increases contact normal anisotropy suggesting that contact normal fabric is dominant in cyclic loading.
The similarity in cyclic behaviour of LRig and T1 indicates that scaled laboratory element tests are capable for reproducing the particle scale behaviour observed in full scale material.
Development and characterisation of DEM particles for modelling railway ballast

4.1 Introduction

The importance of particle shape properties in the mechanical response of a coarse granular system have been demonstrated by many authors (Cho et al. 2006; Mirghasemi et al. 2002; Jensen et al. 2001; McDowell & Li 2011; Nougier-Lehon et al. 2003). Even so, the use of spheres as idealised particle geometry in Discrete Element Method (DEM) simulations within the realm of geomechanics remains popular (O'Sullivan 2011).

To overcome the quantitative shortcomings of spheres, a number of alternative particle geometries have been proposed. The most commonly used include ellipsoids and sphere clusters/agglomerates (e.g. Ferrellec & McDowell 2010). The technique known as “potential particles” (Houlsby, 2009; Harkness, 2009) makes possible the modelling of strictly convex particles, based on polyhedral forms with slightly rounded corners, edges and faces.

With developments such as potential particles and agglomerates allowing the modelling of non-regular particle geometry more usually seen in nature, there is
a need to relate DEM particles to real soil from a morphological perspective. When simulating real materials both the particle sizes and shapes should be considered. This chapter contributes to this aim by developing shape characterisation techniques for railway ballast, and then constructing a library of DEM particles that are quantitatively related in terms of shape to real ballast.

**Notation**
Quantification of particle form requires the measurement of the major dimensions of a particle which for a cuboid are the length, breadth and height. A number of different notations have been used historically to refer to these three measurements.

![Diagram showing different notations for dimensions of an object](image)

*Figure 4.1 Different notations used to identify the dimensions of an object*

These include $D'$, $D''$ and $D'''$ (Wentworth 1922a) $a$, $b$ and $c$ (Zingg 1935; Krumbein 1941; Pettijohn 1975) and $L$, $I$ and $S$ (Sneed & Folk 1958). Figure 4.1 illustrates these notations. Although not always explicitly stated in the past, most authors have agreed that all three dimensions should be orthogonal, although they need not intersect at a common point (Flemming 1965; Sneed & Folk 1958).

For the purposes of the work presented here, Sneed and Folk’s notation (Sneed & Folk 1958) will be adopted. $L$ (longest) will be assigned to the longest dimension of the particle, $I$ (intermediate) being the intermediate dimension perpendicular to $L$ and $S$ (smallest) being the shortest dimension perpendicular to both $L$ and $I$. 

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4.2. Particle characterisation using digital imaging

At its most basic, a steel tape or ruler can be used to measure the dimensions of the particles manually and compute shape parameters (Wentworth 1922b). Krumbein (1941) used a sliding rod caliper, shown in Figure 4.2, for measuring the diameters of pebbles. More recently, Jahn (2000) built a device consisting of a digital caliper connected to a data logger and a computer (Figure 4.3). A particle is placed on a press table, and the press is lowered until it touches the aggregate particle and stops. The device records the gap between the press and the table, which is equal to the particle dimension. The particle is then rotated into another orientation and the procedure is repeated to obtain other dimensions. These readings are recorded in a customised spread sheet that computes the dimensional ratios in the aggregate specimen.

![Figure 4.2 Sliding rod caliper (Krumbein 1941)](image)

The manual methods previously described are usually easy to deploy and tend to be of low capital cost. However, the repeatability of these methods, especially in
multiple-operator situations, is questionable. Experiments conducted by Blott (2008) have indicated that, in the case of measurements made by a single operator on gravel particles using calipers and a ruler, the average error lies in the range of 0.5% to 3.3%. The precision becomes significantly worse for multiple-operator situations where the average error ranged from 1.7% to 6.3%. While the capital investment associated with manual measurements methods is not very high, they are highly time consuming and therefore labour intensive. The overall cost can therefore be considerably high. The combination of high labour cost and poor reproducibility of manual methods have led to significant advances in automated direct measurement techniques.

Modern automated methods of direct measurements mainly use a digital imaging system coupled with a computer program to capture and analyse aggregate shape characteristics.

In the following section, the state of the art in image acquisition, processing and analysis will be outlined.

4.2.1. Image acquisition

When characterising medium to coarse gravels (i.e. 6.3-100mm (Powrie 2004)) using image based methods, all popular techniques involve the use of a Charge-Coupled Device (CCD) to capture a digitised image of the specimen. The various techniques reported in the literature can be divided into three categories; laser scanning/profiling, dynamic video capture and stills imaging. A brief description of each is given below. Recently, the use of X-ray computed tomography (CT) has also been noted in the literature (e.g. Masad et al. (2005)). However, the high cost associated with it has meant that this technique remains relatively inaccessible and is not considered here.

Laser scanning

Laser scanner or laser surface profilers use a laser source that projects a laser stripe on the surface of the object to be measured, while one or more cameras capture the reflection. As the position of the camera with respect to the laser source is known, mathematical transformations can be used to calculate the three dimensional coordinates of the projected laser strip at a given resolution.
(Valkenburg & McIvor 1998). As the laser scans over the object, a three dimensional cloud of data points representing the scanned surface is generated. This data cloud is then used to determine the 3D geometrical properties of the object.

A number of authors have utilised this technique for the characterisation of particles. Kim et al. (2001) developed the Laser-based Aggregate Scanning System (LASS) that has a laser scanner mounted on a linear motion slide allowing it to pass over an aggregate specimen while scanning it with a vertical laser plane (Figure 4.4). Kim (2002) showed that the LASS system was capable of scanning 6000 particles per hour, or was approximately 150 times faster than manual measurements using a caliper. The high output rate is achieved partly because scans are carried out along one axis only (in this case the vertical). As a result, only a partial scan of the particle is possible since the laser plane is unable to reach the shadow region as shown in Figure 4.5. Consequently, it is assumed that dimension of the particle in line with the scanning axis (d) is equivalent to the distance from the top of the particle to the scanning platform.

A complete 3D scan of a particle is possible by manually rotating either the particle (Illerstrom 1998) or the laser scanner (Lanaro et al. 2002; Tolppanen et al. 2002) by 90° around its vertical axis and rescanning the particle. However this effectively doubles the scan time and introduces additional post processing that is needed to align the two separate scans.

Dynamic imaging

This is perhaps the most popular and well known method of acquiring raw image data for particle characterisation. Early video based particle characterisation used the principle of shadowgraph (Descantes et al. 2006; Caussignac et al. 1985) to capture a silhouette of a particle that passes between a light source and an imaging plane as it falls. ISO 13322-2:2006 provides guidance for measuring and describing particle size distribution using image analysis methods where particles are in motion (ISO, 2006).
The first device to use this method, the VDG 40 Videograder, was developed in France by the Laboratoire Central des Ponts et Chaussées (LCPC) (Weingart & Prowell 1998; Descantes et al. 2000). The system consists of a mechanism to feed the aggregates so that they fall in between a light source and a linear charge-coupled device (CCD) camera. A schematic of the system is given in Figure 4.6.

The camera scans the falling particles at a frequency of 13kHz (Descantes et al. 2006) and successive scan segments are assembled in sequence to form a pseudo-image (Weingart & Prowell 1998) as shown in Figure 4.7. Since the VDG 40 captures only one view of a particle, 3D measurements are extrapolated by assuming that the particle is a rotational ellipsoid (Figure 4.8), and the captured shadow is assumed to be the projection of the ellipsoid on a plane containing its larger axis (Bouquety et al. 2006).
A number of other commercially available devices have also implemented this
technique such as the Computer Particle Analyser (W.S. Tyler), OptiSizer PSDA
5400 (Micromeritics), Video Imaging System (John B. Long Co. Video) and the
Particle Size Distribution Analyzer by Buffalo Wire Works (Browne et al. 2001).

While shadowgraph based image acquisition is fast and tends to have a very high
output, it is mainly intended for providing the gradation curves (particle size
distributions) of granular mixtures and not the aspect ratios of individual particles
(Tutumluer et al. 2000).

Attempts have been made to estimate the third dimension as mentioned before.
However, many have proved to be highly unreliable since individual particle
masses were unknown and an average was used.

Given these shortcomings, many authors have developed video methods that
include two or more mutually orthogonal cameras imaging the same particle,
allowing the gathering of 3D information on the particle (e.g. Tutumluer et al.

To allow for rapid image acquisition, individual particles are dropped on to a
conveyor belt (or an alternative) which transports them past the view of the
cameras. Owing to the moving nature of the aggregates on the conveyor,
progressive scan type video cameras are usually used. The University of Illinois
Aggregate Image Analyser (UIAIA) (Tutumluer et al. 2000) and WipShap (Maerz
& Zhou 1999) are examples of setups that make use of this technique.

**Digital still imaging**

Rectangular CCD cameras are used to capture an image of the particle placed on
a surface normal to the line of sight of the camera. Most of the experimental
setups described in the literature use the CCD camera in a downward pointing
position, overhanging the sampling area (Figure 4.10).
Figure 4.6 Schematic of the VDG 40 (LCPC 2012)

Figure 4.7 Imaging frequency

Figure 4.8 Rotational ellipsoid

Figure 4.9 University of Illinois Aggregate Image Analyser (left) and WipShape (right)
While a setup of this type is very easy to implement, it is only capable of acquiring a 2D projection of the particle. To overcome this limitation, researchers have attached aggregates to transparent specimen trays that have two perpendicular faces, one with an adhesive surface (Figure 4.11). After the initial projected image of the aggregates has been captured, the specimen trays are rotated 90 degrees so that the aggregates are now perpendicular to their original orientation. This allows the projection in the third dimension of the aggregate to be captured (Frost & Lai 1996; Kuo et al. 1996; Kuo et al. 1998). Alternatively, a projection of the third dimension of the particle can be obtained by using an additional camera placed orthogonal to the downward pointing camera (Frost & Lai 1996).

Figure 4.10 Image acquisition using one camera (Kwan et al. 1999)

Figure 4.11 Perspex specimen tray (Frost & Lai 1996)
4.2.2. Image processing

Numerous enhancement and corrective processes can be applied to an image prior to analysis. The most commonly used are briefly described below.

**Non-uniform lighting correction**

Simple brightness thresholding is by far the easiest and fastest method of isolating features in an image, however it is important to consider the problem of shading of images. It is not always possible to ensure that the lighting of the specimen in the field of view is absolutely even. Depending on the application, an uneven light distribution may require filtering. In many cases, the effects of an uneven light distribution can be filtered out of the image sufficiently to allow further image processing.

Perhaps the simplest solution is to acquire a background image in which a uniform (coloured or textured) reference surface or specimen is viewed in place of the actual specimens to be imaged and the light intensity recorded. This image can then be used to level the brightness in subsequent images. However, finding an appropriate reference object for this purpose can be a matter of trial and error. In practice, the spatial variation in colour values registered by the camera depends not only on the strength and type of illumination (Lamoureux & Bollmann 2005), but also on the reflectivity and the colour intensity of the imaged objects (Nederbragt & Thurow 2005). Alternatively, the uneven light distribution can be estimated for the image to be corrected by selecting a number of points in the image, a list of brightness values and locations is acquired. These are used to perform least-squares fitting of a function B(x,y) that approximates the background and can be levelled just as a physically acquired background image would be.

In the process of levelling one image by using a different image as reference, some of the dynamic range of the original data is lost. The greater the variation in background brightness, the less the remaining variation from that level can be recorded in the image and retained after the levelling process. This loss, and the inevitable increase in statistical noise that results from subtracting one signal from another, require that all practical steps should be taken to make the illumination
uniform and reduce noise when acquiring the images, before resorting to processing methods.

**Contrast and brightness correction**

Visual inspection of the images is usually an important part of image analysis, to determine the most suitable method for the processing of the data set. However, visual identification of the relevant features can be difficult if the image is dark, or if the difference in colour between the various components is small. If this is the case, contrast and brightness can be enhanced after acquisition, in such a way that the required information remains unchanged while features of interest are made more clearly visible.

The contrast or brightness of an image can be adjusted by contrast stretching. This is sometimes referred to as normalisation. The simplest contrast stretch is a linear transform that maps the lowest grey-level in the image to zero and the highest to 255 (for an 8bit image), with all other grey levels remapped linearly between zero and 255 to produce a high-contrast image that spans the full range of grey levels.

The linear transform for contrast enhancement spreads the grey-level values evenly over the full contrast range available; thus the relative shape of the histogram remains unchanged but it is widened to fill the range; an example can be seen in Figure 4.12. The stretching of the histogram creates evenly distributed gaps between grey-level values in the image. Although the linear transform will increase the contrast of the image, the steps between the populated grey-level values increase in contrast as well, which can result in visible contouring artefacts in the image.

**Noise reduction**

In filtering noise from images, the underlying assumption is that a single pixel in an image is much smaller than any important detail within that image; hence a neighbouring pixel is likely to belong to the same domain. This allows for some form of averaging between neighbouring pixels to reduce random noise.
A number of studies have evaluated various types of filters to determine optimal noise reduction while maintaining most of the details (e.g. Starkey 1991; Russ 2011). In most cases the filters consist of a square array of numbers (a kernel, with dimension 3 x 3, or 5 x 5, etc.), which forms a multiplier that is applied to each pixel and its adjacent neighbours. This array is moved pixel by pixel across the entire image. The filter replaces the intensity of the central pixel with the average of the value. Averaging filters, however, have disadvantages, particularly when details such as grain boundaries are of interest. Because several pixel values are averaged, boundaries are typically blurred and can be displaced relative to the original position, while the noise remains visible. Further, these types of filters can also create "pseudo resolution" in that the filtering process produces artificial domains, or connections between originally discrete regions. Consequently, average noise filtering is usually the least desirable solution, because it is an irreversible operation.

Related filters, known as median filters and hybrid-median filters, find the median value of a pixel and its adjacent neighbours after ranking these values. The filter then replaces the original pixel value with the median value. This process is particularly good for removing pixel-scale noise and has the added advantage of not displacing or blurring distinct boundaries, so that these filters can be applied repeatedly (Huang et al. 1979). Because it discards the extreme values, a median filter is often more successful in removing noise without substantially altering the information in the image.
Colour space conversion

Colour can be expressed in a number of different coordinate systems designed for various applications. Colour in digital images is expressed in red, green, and blue (RGB) colour coordinates, which is the system used for televisions and computer screens. However, the RGB system is not the most suitable for presentation of colour data for image processing. Indeed, the two important features for visual classification of a colour are hue or tint (e.g., green) and lightness (e.g., dark green or light green). In RGB, each of the three co-ordinates is a combination of lightness and hue. Shades of grey are expressed by R = G = B, with black (R = G = B = 0) and white (R = G = B = 255) as the two extremes. The hue of a colour is determined by difference between the values of R, G, and B. As a result, it is difficult to interpret the actual colour of an object from a plot of R, G, and B values.

The L*a*b* colour coordinate system is more appropriate to present colour information (or lightness/grey-scale) in numerical values, because it is designed to match human colour vision. The L*a*b* colour system is defined by the Commission Internationale de l’Éclairage (CIE L*a*b*), the asterisks differentiate this system from its predecessor CIE Lab. The L*a*b* space consists of a luminosity 'L*' or brightness layer, chromaticity layer 'a*' indicating where colour falls along the red-green axis, and chromaticity layer 'b*' indicating where the colour falls along the blue-yellow axis. Both a* and b* are zero when a colour is grey.

The inherent advantage of this colour space lies in its ability to isolate the luminosity 'L*' or brightness from the colour information making it easier to segment images that have uneven lighting across the frame or between images (a particular pitfall for Greyscale and the RGB colour space). This means that a fixed segmentation colour value can be used across many images with great effect, making automation easier.

The transformation from RGB to L*a*b* requires an intermediate step, called CIE XYZ (Russ, 2011):
\[
\begin{bmatrix}
X \\ Y \\ Z
\end{bmatrix} = 
\begin{bmatrix}
0.4124 & 0.3576 & 0.1805 \\
0.2126 & 0.7152 & 0.0722 \\
0.0193 & 0.1192 & 0.9505
\end{bmatrix} \cdot 
\begin{bmatrix}
R \\ G \\ B
\end{bmatrix}
\] (4.1)

Based on these XYZ values, the L*, a*, b* components are:

\[
L* = 116 \cdot f\left(\frac{Y}{Y_n}\right) - 16
\]

\[
a* = 500 \cdot \left[f\left(\frac{X}{X_n}\right) - f\left(\frac{Y}{Y_n}\right)\right]
\]

\[
b* = 200 \cdot \left[f\left(\frac{Y}{Y_n}\right) - f\left(\frac{Z}{Z_n}\right)\right]
\] (4.2)

The function \(f\) is defined as:

\[
f(q) = q^{\frac{1}{3}}
\] (4.3)

if \(q\) is greater than 0.008856, otherwise:

\[
f(q) = 7.787 \cdot q + 0.137931
\] (4.4)

\(X_n, Y_n, Z_n\) are calculated for a reference white point that depends on the illumination of the scene.

Conversion from RGB values to greyscale values can be achieved by forming a weighted sum of the R, G, and B components (Russ, 2011):

\[
0.2989 \cdot R + 0.5870 \cdot G + 0.1140 \cdot B
\] (4.5)

**Colour based segmentation**

Colour based segmentation is usually carried out by using a \(k\)-mean cluster algorithm where the Euclidian distance (in a given colour space) for a pixel is compared with a given reference (or segmentation) value and tolerance. Based on this, individual pixels can then be grouped as either features of interest or a background. Figure 4.13 illustrates this process. It should be mentioned that images that have been segmented using methods other than thresholding will have to go through that process in order to be binarised as explained below.
**Binary image processing**

Grey-level thresholding results in an image (or mask) where a pixel can only have a value of 0 or 1. This is why such images are referred to as binary images. The accepted convention is to have the feature of interest represented by ‘1s’ and the background by ‘0s as is shown in Figure 4.13(C).

![Binary Image Processing Diagram](image)

*Figure 4.13 Colour based segmentation is used to isolate pixels that are reddish in colour (A) and remove or ‘switch off’ all other pixels (B). Binarisation of segmented image (C)*

The simplicity of binary images lends itself well to computer vision and allows a number of important morphological operations to be carried out. These include (but are not limited to) erosion, dilation, hole-filling, distance maps, skeletonisation, watershedding and edge detection. For detailed explanations of these and other morphological operators, the interested reader is directed to image processing textbooks e.g. Nixon & Aguado (2012); Russ (2011); Umbaugh (2005).

**Spatial calibration**

When images are used as a means of analysing the geometrical properties of an object, it is important that the measurements are properly calibrated so they are accurate and reproducible. This is especially true when data from different sources are compared. Spatial calibration is carried out by determining the number of pixels that make up a known length in an image and thus the actual scaled size/length of a pixel in SI units.

It is important that spatial calibration is carried out every time the image acquisition parameters (e.g. camera, lens, focal length/magnification, etc.) change so that comparisons are still valid between datasets.
4.2.3. Image Measurement methodology

**Area measurements**

Area is defined as the measure of a planar surface in 2-D space. It was proven by Minkowski (1903) that this measure is readily accessible without bias by counting the number of squares ($N$) on a systematic grid. The grid spacing in the horizontal ($s_h$) and vertical ($s_v$) directions defines the elementary surface area ($s$) to be associated with each pixel:

\[ s = s_h \times s_v \]  \hspace{1cm} (4.6)

Hence, we get:

\[ A = N \times s \]  \hspace{1cm} (4.7)

Area measurements defined in this way are robust against translation and rotation of the grid of pixels, which is a very important attribute. The precision of the estimation is a function of the density of the pixel grid so that increasing image resolution will also improve the approximation of the area.

**Diameter measurements**

Particle size, in the sense commonly used, is a linear length measure, measured in meters $m$. In this sense it can be uniquely defined only for spheres, where it equals the diameter (or radius). For all other shapes, particle size must be clearly defined via the measuring procedure used. Given that most naturally occurring particles are anisometric i.e. they have significantly different extensions in different directions, at least three linear length measures are needed to describe the size and shape of such particles satisfactorily.

So called derived diameters are determined by measuring a size-dependent property of the particle and relating it to a single linear dimension.

**Equivalent disc diameter**

Differences in shape or orientation can make it difficult to judge relative size. It is therefore convenient to quantify size using the diameter of a disc having the same area $A$ as the particle. This equivalent disc diameter $D_{eq}$ offers an easily comparable parameter to characterize size.
The equivalent disc diameter $D_{eq}$ is obtained by arranging the classical formulae for computing the surface of a disc into:

$$D_{eq} = \sqrt{\frac{4 \cdot A}{\pi}}$$  \hspace{1cm} (4.8)

The main practical advantages of $D_{eq}$ is that it does not require any additional computation with respect to the area and that it provides a convenient linear measure that ignores any details of shape. However, it should be understood that the same comments would apply if all particles were considered as squares and $D_{eqS} = \sqrt{A}$ as used in the computation of an equivalent square side $D_{eqS}$.

In practice, the use of an equivalent diameter should be restricted to the analysis of a set of objects with very similar shapes (Francus 2004).

**Inscribed and circumscribed circle diameters (ICC)**

Wadell (1935) described a method of fitting circles to the outline of quartz particles to measure their minimum and maximum diameters. The maximum diameter $D_{max}$ is that of the smallest circle that is capable of completely enclosing the particle. The minimum diameter $D_{min}$ is that of the largest circle that may be completely enclosed within the boundary of the particle. Figure 4.14 illustrates this concept.

![Figure 4.14 Inscribing and circumscribing circles defining $D_{min}$ and $D_{max}$.](image)

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Equivalent inertia ellipse diameters (EIE)

Medalia (1971) proposed a diameter estimation based on a simplified shape model which relies on the computation of the real moments of inertia of the object and the mathematical derivation of an ellipse sharing the same inertial properties. This ellipse can be characterized by its major ($D_{\text{max}}$) and minor ($D_{\text{min}}$) diameters its centre of gravity and orientation.

The moments of inertia of the shape coordinates are given by:

\[
I_{xx} = \frac{1}{n} \sum (x_i - \bar{x})^2 \\
I_{yy} = \frac{1}{n} \sum (y_i - \bar{y})^2 \\
I_{xy} = \frac{1}{n} \sum (y_i - \bar{y})(x_i - \bar{x})
\]

(4.9)

The lengths of the axes of the ellipse of equivalent inertia are:

\[
D_{\text{max}} = 4\sqrt{\alpha + \beta} \\
D_{\text{min}} = 4\sqrt{\alpha - \beta}
\]

(4.11)

Figure 4.15 Equivalent inertia ellipse
where:

\[
\alpha = \frac{1}{2}(I_{xx} + I_{yy})
\]

\[
\beta = \sqrt{\alpha^2 - I_{xx}I_{yy} + I_{xy}}
\]

Finally, the orientation \(\theta\) of the major axis is given by:

\[
\theta = 90 - \frac{180}{\pi}\tan^{-1}\left(\frac{I_{xx} - \alpha - \beta}{I_{xy}}\right)
\]

This method of ellipse fitting essentially equates the second moments of area of the actual shape and the equivalent ellipse (Jain 1988) and is considered to be a robust method of measuring the geometrical properties of arbitrary shaped particles (ISO 2008). EIE is a region based method that uses the moments of a shape in estimating an equivalent ellipse (ISO 2008; Francus 2004; Jähne 1995; Jain 1988; Russ 2011). It is therefore unable to take into account the irregularities common with anisometric particles (Mulchrone & Choudhury 2004).

**Feret diameters**

This follows the physical concept of feret/caliper diameter i.e. the distance between two parallel tangents. In image analysis, the simplest implementations involve calculating the maximum Euclidian distance between two pixels (on the boundary of the particle) in the x and y direction. This is sometimes referred to as a bounding box/square measurement since it is analogous to fitting a box to the particle as shown in Figure 4.16 (A).
Measurements made this way suffer from a lack of robustness since any degree of rotational transformation of the axes will change the measured length between measurements. This effect can be seen in Figure 4.16 (B) where the particle from the previous figure has been rotated by 45° resulting in a large change in the measure of lengths $D_1$ and $D_2$.

To overcome the limitations caused by orientation, the feret diameter is usually computed for a discrete set of orientations (typically 8 or 16) and from this the maximum and minimum feret diameters are determined (Pirard 2004). Figure 4.17 illustrates the process.
However it should be noted that the direction of the maximum feret is in itself not a very robust notion since a very slight perturbation of the surface profile (of the particle) is capable of turning the maximum feret direction by 90° (Francus 2004). As a result, the number of orientations would have to equal the number of pixels making up the boundary of the particle which could be computationally expensive.

**Perimeter**

The perimeter of a feature is a well-defined geometrical parameter that is easily computed in continuous real space (Russ 2011). However, in pixelated images, where the feature occupies what is effectively a mosaic of discrete squares (or grid space), it becomes a complex problem.

For a curve enclosing a region $S$ and described by a set of parametric coordinates $x(t)$ and $y(t)$, the perimeter of the region can be defined by:

$$ P(S) = \int x^2(t) + y^2(t) \, dt \quad (4.13) $$

This equation is the summation of all the infinitesimal arcs that define the curve (Nixon & Aguado 2012). In the case of a digitised image, $x(t)$ and $y(t)$ are defined by the pixels that make up the feature/curve. As such the perimeter can be approximated by:

$$ P(S) = \sum \sqrt{(x_i - x_{i-1})^2 + (y_i - y_{i-1})^2} \quad (4.14) $$

Given that the pixels (in an image) are organised in a square grid, the value of the summation terms $(x_i, y_i)$ and $(x_{i-1}, y_{i-1})$ are determined by the type of pixel connectivity (or connectedness) that is used to isolate the boundary of the feature. Figure 4.18 shows a diagrammatic representation of pixel connectivity.

If a Four-way connectedness (4-c) is used, the summations terms are equal to 1. However, this can lead to an overestimation of the perimeter. Therefore, the
Eight-way connectedness (8-c) where the diagonal distant is $\sqrt{2}$ is preferred (Nixon & Aguado 2012).

![Diagram of pixel connectivity](image)

*Figure 4.18 Types of pixel connectivity. Left: four way connectedness, 4-c. Right: Eight way connectedness, 8-c.*
4.3. Method

4.3.1. Specimen preparation

The railway ballast used in this experiment was sourced from the Cliffe Hill Quarry in Leicestershire operated by Midland Quarry Products. The ballast from this source is of the Granodiorite type in the Igneous group and is crushed to comply with BS EN 13450:2002 grading category A (MQP 2013). To ensure that the material was within specification, a particle size distribution (PSD) analysis was carried out in compliance with BS 1377-2: 1990. 120 kg of material was sieved and the results from the PSD analysis are shown in Table 4.2 and Figure 4.19.

<table>
<thead>
<tr>
<th>Table 4.1 Network rail ballast specification (BS EN 13450:2002)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sieve size mm</td>
</tr>
<tr>
<td>Grading category</td>
</tr>
<tr>
<td>----------------</td>
</tr>
<tr>
<td>80</td>
</tr>
<tr>
<td>63</td>
</tr>
<tr>
<td>50</td>
</tr>
<tr>
<td>40</td>
</tr>
<tr>
<td>31.5</td>
</tr>
<tr>
<td>22.4</td>
</tr>
<tr>
<td>31.5 to 50</td>
</tr>
<tr>
<td>31.5 to 63</td>
</tr>
</tbody>
</table>

NOTE 1 The requirement for passing the 22.4 mm sieve applies to railway ballast sampled at the place of production.

NOTE 2 In certain circumstances a 25 mm sieve may be used as an alternative to the 22.4 mm sieve where a tolerance of 0 to 5 would apply (0 to 7 for category F).

<table>
<thead>
<tr>
<th>Table 4.2 Particle size distribution analysis of Cliffe Hill ballast specimen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle Size (mm)</td>
</tr>
<tr>
<td>------------------</td>
</tr>
<tr>
<td>63</td>
</tr>
<tr>
<td>50</td>
</tr>
<tr>
<td>40</td>
</tr>
<tr>
<td>31.5</td>
</tr>
<tr>
<td>22.4</td>
</tr>
<tr>
<td>&gt;22.4</td>
</tr>
</tbody>
</table>
100 ballast particles were picked at random to make up the specimen used for the purposes of shape characterisation. The specimen was then washed to remove the dust and debris on the surface of the particles. Once dry, each of the particles was numbered to allow identification.

4.3.2. Image acquisition

The method developed uses 3 cameras to collect images of individual aggregate particles from three orthogonal directions and in essence capturing a 3D view of each particle as shown in Figure 4.20 and Figure 4.21. A three sided stage was constructed from plywood to serve as the backdrop for each of the three views and a cylindrical piece of wood was used as a prop for placing the particles (Ahmed et al. 2014). To segment the particle from the background, the stage and prop were painted green. This is because image sensors in digital cameras are most sensitive to green, due to the Bayer pattern allocating more pixels to the green channel. Therefore, the green camera channel contains the least "noise" and can produce the cleanest segmentation. Lighting was controlled using three continuous light sources to eliminate shadows and illuminate the particle evenly. While there is a multitude of image enhancement and correction tools available (Section 4.2.3) it is best practice to minimise and if possible eliminate undesirable artefacts at the acquisition stage. This reduces computational costs and avoids uncertainties associated with correction algorithms such as noise reduction.

During image capture, ballast particles were placed on the prop one at a time and the three synchronised cameras triggered to simultaneously capture the images of the front, top, and side views of the particle. This process was then repeated for other particles. After the initial equipment setup and specimen preparation, it took approximately 10 seconds to place a particle on the stage, capture the images and remove it from the stage. 100 particles were imaged in this way taking approximately 16 minutes.
Figure 4.19 Particle size distribution graph for Cliffe Hill

Figure 4.20 Schematic drawing of camera positions.

Figure 4.21 Setup of cameras and background.
4.3.3. Image processing

A Matlab routine was written to carry out the image processing and subsequent analysis automatically. As a first step, all the acquired images were converted from RGB to L*a*b* colour space. To perform colour-based segmentation (as described in Section 4.2.2) a reference colour value of the background and the ballast is needed. This was done by sampling two representative areas of an image picked randomly from the set to be analysed as shown in Figure 4.22. The measured colour values were then used in the $k$-mean clustering algorithm for all the images in the set.

Figure 4.23 illustrates the segmentation process where the green background (B) and the ballast particle (C) are separated into two images from the original image (A).

The final step in the processing involved the binarization of the image where the pixels of the colour image of the particle were stored as a single bit (0 or 1) as shown in Figure 4.24A.

![Sampling image for colour reference](image1)

**Figure 4.22 Sampling image for colour reference**

![Colour based segmentation. A) The original image. B) The background. C) The particle.](image2)

**Figure 4.23: Colour based segmentation. A) The original image. B) The background. C) The particle.**
For the purposes of diameter measurement, the boundary of the particle (in the binary image) is traced and a set of Cartesian coordinates (in 2D space) are retrieved for each pixel that make up the particle outline.

4.3.4 Dimension estimation using Geometric Best-fit Ellipse (GBE)

A new method of estimating the diameters of particles using a geometric best fit ellipse is proposed.

This boundary based method considers the outline of the particle as a set of discrete points to which an ellipse is fitted with the aim of minimising the distance between the points that make up the particle boundary and the fitted ellipse while preserving the area. This is essentially a curve fitting problem that is typically solved by using the Least Squares (LS) method. There are two main categories of LS fitting problems for geometric features, algebraic and geometric fitting, differentiated by their respective definition of the error distances involved (Sampson 1982; Pearson 1901; Ahn et al. 2001).

While algebraic fitting has distinct advantages in implementation and computing costs, the approximation of the algebraic distance has a bias towards low curvature points rather than high curvature points, leading to inaccurate geometric interpretation of the fitting parameters and error distances (Rosin 1993).

On the other hand, in geometric fitting the error distances are defined with the orthogonal, or shortest, distances from the given points to the geometric feature to be fitted. This is preferred in graphical and image applications.
Gander et al. (1994) proposed a geometric ellipse fitting algorithm in parametric form where the following equation is considered:

$$\mathbf{x} = \mathbf{z} + \begin{pmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{pmatrix} \cdot \begin{pmatrix} a \cos \varphi \\ b \sin \varphi \end{pmatrix}$$

(4.15)

Where $\mathbf{x} = (x_1, x_2)^T$ is the coordinate vector for a given point $P$ and $\mathbf{z} = (z_1, z_2)^T$ is the centre of the ellipse.

To minimise the sum of squared distances for a set of points to best fit ellipse, the solution to the following nonlinear least squares problem is required:

$$\mathbf{g}_i = (x_{i1}, x_{i2}, z_1, z_2) - \begin{pmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{pmatrix} \cdot \begin{pmatrix} a \cos \varphi \\ b \sin \varphi \end{pmatrix} \approx 0, \quad i = 1, \ldots, m.$$  

(4.16)

Resulting in $2m$ nonlinear equations for $m+5$ unknowns ($\varphi_1, \ldots, \varphi_m, \alpha, a, b, z_1, z_2$).

The initial guess is calculated by a linear least squares routine, by using the Bookstein constraint (a constraint that guarantees that the obtained coefficients are invariant to rotation and translation of the curve), which is then used in a Gauss-Newton algorithm (Boyd, 2007; Gill et al., 1982) to solve a sequence of linear least squares problems iteratively. A Matlab script was written to implement the algorithm presented above to allow automated ellipse fitting (see Appendix D.1).

### 4.3.5. Shape parameters used

As described in the literature review, characterisation of a particle involves the quantitative analysis of its Form, Angularity and Roughness. However, it is common practice to model the roughness of particles (or material) as inter-particle friction in a contact constitutive model. As such, only the Form and Angularity of the particle will be considered.

**Form**

For the purposes of Form characterisation, only three measurements are needed, the shortest (S), intermediate (I) and longest (L) diameter of a particle.
It is assumed that the longest and intermediate diameters lie parallel to the largest projected area of a particle (Wadell 1933; Malvern-Instruments 2005; Sneed & Folk 1958), and the smallest is perpendicular to the largest projection plane.

Using the three diameters, three first order Form ratios can be calculated:

\[
\text{Elongation} = \frac{I}{L} \\
\text{Flatness} = \frac{S}{I} \\
\text{Equancy} = \frac{S}{L}
\]

(4.17)

All three measures can range between 0 and 1.

I/L approaching ‘0’ indicates a highly elongated object I/L approaching ‘1’ indicates a highly ‘disc like’ object.

S/I approaching ‘0’ indicates a form that is almost 2D (e.g. paper) whilst, a value approaching ‘1’ indicates increasing depth.

An S/L value of ‘1’ would indicate a perfectly equant (e.g. sphere or cube) form. Values closer to ‘0’ indicate a shape that is highly ‘non-equant’ or non-spherical (e.g. a Biro pen S/L =0.05).

Angularity

Since the Form of a particle is defined by an ellipse, it seems logical to define Angularity as a measure of how much a particle’s perimeter deviated from the ideal shape describing its form.

A new angularity measure, based on the perimeter of the particle and the perimeter of its GBE, is proposed:

\[
\text{Ellipseness } (E) = \frac{P_E}{P_o}
\]

(4.17)

where \(P_o\) is the perimeter of the particle and \(P_E\) is the perimeter of the GBE for that particle. Ellipseness \(E\) can range from 0 to 1 and as the particle becomes more elliptic.
4.4. Shape characterisation of ballast

4.4.1. Verification of proposed GBE

To verify the applicability of the proposed diameter measurement method, a comparison is made between the proposed method of geometric best fit ellipse, existing image based methods (i.e. inscribed/circumscribed circle diameters (ICC) and equivalent inertia ellipse diameters (EIE)) and manual measurements.

The longest (L), Intermediate (I) and Shortest (S) diameters of 20 randomly selected ballast particles were measured using a digital caliper with a precision of 0.01\(mm\). To ensure consistency of measurement between particles, the routine described by Krumbein (1941) was followed. The steps are:

1. The longest possible caliper length of the particle is determined.
2. The particle is then held between the thumb and forefinger by the ends of this longest diameter, and rotated until the largest section is seen by the eye. (This is equivalent to finding the position in which the pebble would cast its largest shadow in a parallel light beam.)
3. The widest length, orthogonal to the longest diameter, is measured. This is the intermediate diameter.
4. With the particle still held by its long diameter, the maximum projected plane is rotated to a vertical position, which places the short diameter in a horizontal plane.
5. The widest part of the particle in the horizontal plane is measured, also perpendicular to the long axis. This is the shortest diameter.

*Figure 4.25 Manual measurement of particle diameters (Krumbein 1941)*
Comparisons of the three dimensions (L, I and S) determined using manual measurement and the three different image analysis methods are done by plotting each image based method against the manual measurements as shown in Figure 4.26 to Figure 4.28. An \( x = y \) line is plotted in these figures as a means of visualising the deviation of the manual measurements from the image based ones.

<table>
<thead>
<tr>
<th></th>
<th>L</th>
<th>I</th>
<th>S</th>
</tr>
</thead>
<tbody>
<tr>
<td>Manual</td>
<td>65.53</td>
<td>49.48</td>
<td>30.18</td>
</tr>
<tr>
<td>GBE</td>
<td>-3.29%</td>
<td>-5.62%</td>
<td>0.09%</td>
</tr>
<tr>
<td>ICC</td>
<td>2.60%</td>
<td>-11.64%</td>
<td>-1.57%</td>
</tr>
<tr>
<td>EIE</td>
<td>-4.61%</td>
<td>-5.61%</td>
<td>3.00%</td>
</tr>
</tbody>
</table>

The arithmetic mean is commonly used as a measure of a dataset’s central tendency. Table 4.3 summarises the variation in the mean of the three different measurement methods to that of the manual measurements. Negative numbers indicate an underestimation from the mean of the manual measurement while a positive number indicates an overestimation.

To quantify the deviation of the image based methods from the manual one, the coefficient of determination \( R^2 \) can be calculated using:

\[
R^2 = 1 - \frac{SS_{err}}{SS_{tot}} 
\]

(4.18)

where \( SS_{err} \) is the sum of the squared residuals:

\[
SS_{err} = \sum (y_i - \hat{y}_i)^2
\]

(4.19)

\( y_i \) is the observed data set (image-based) and \( \hat{y}_i \) is the associated modelled value (manual). And \( SS_{tot} \) is the total sum of squares proportional to the specimen variance:

\[
SS_{tot} = \sum (y_i - \bar{y})^2
\]

(4.18)

where \( \bar{y} \) is the mean of the data set. \( R^2 \) is equal to 1 when \( SS_{err} \) is equal to zero, i.e. all points fall on the \( x = y \) line indicating that there is no variation in the
measurement methods (Mendenhall & Sincich 2006). A summary of the $R^2$ values can be found in Table 4.4.

<table>
<thead>
<tr>
<th></th>
<th>L</th>
<th>I</th>
<th>S</th>
</tr>
</thead>
<tbody>
<tr>
<td>GBE</td>
<td>0.942</td>
<td>0.906</td>
<td>0.921</td>
</tr>
<tr>
<td>ICC</td>
<td>0.973</td>
<td>0.606</td>
<td>0.946</td>
</tr>
<tr>
<td>EIE</td>
<td>0.915</td>
<td>0.891</td>
<td>0.929</td>
</tr>
</tbody>
</table>

It is not surprising to see that the ICC method is the best performer when estimating the longest diameter L. This is because ICC uses a circumscribing circle to measure this diameter and is effectively equivalent to a feret measurement taken with an infinite number of orientations. It is also the strongest when estimating the smallest diameter. On the other hand, the ICC method is a very poor estimator of the intermediate diameter. Overall, it is clear that the ellipse-based methods are better estimators of all three dimensions. The use of GBE appears to improve the approximation compared with the EIE especially in terms of L and S. While the difference is slight, it can be argued that any improvement, when working with estimates, is a gain. And since the ultimate goal is to use the estimated diameters to calculate Form ratios, errors in the approximation will inevitably be accumulated in the process. It is therefore important to compare Form ratios calculated using the manual and image-based methods to obtain a complete understanding of the errors associated with the diameter approximation and its effects. Figure 4.29 to Figure 4.31 compare the measured and estimated Form ratios.

<table>
<thead>
<tr>
<th></th>
<th>I/L</th>
<th>S/I</th>
<th>S/L</th>
</tr>
</thead>
<tbody>
<tr>
<td>Manual</td>
<td>0.749</td>
<td>0.630</td>
<td>0.463</td>
</tr>
<tr>
<td>GBE</td>
<td>-1.89%</td>
<td>4.80%</td>
<td>3.14%</td>
</tr>
<tr>
<td>ICC</td>
<td>-13.64%</td>
<td>9.96%</td>
<td>-4.27%</td>
</tr>
<tr>
<td>EIE</td>
<td>-1.02%</td>
<td>8.04%</td>
<td>7.50%</td>
</tr>
</tbody>
</table>

Table 4.6 Coefficient of determination ($R^2$) for the form ratios between manual and image based methods.
<table>
<thead>
<tr>
<th></th>
<th>I/L</th>
<th>S/I</th>
<th>S/L</th>
</tr>
</thead>
<tbody>
<tr>
<td>GBE</td>
<td>0.879</td>
<td>0.689</td>
<td>0.720</td>
</tr>
<tr>
<td>ICC</td>
<td>-1.251</td>
<td>0.410</td>
<td>0.805</td>
</tr>
<tr>
<td>EIE</td>
<td>0.831</td>
<td>0.615</td>
<td>0.610</td>
</tr>
</tbody>
</table>

Table 4.5 presents the variation of the mean for the form ratios compared with the manual measurement. The large deviations of the Elongation (I/L) and Flatness (S/I) ratios, using the ICC method are a direct result of its greater inaccuracy in estimating the Intermediate diameter.

This is also seen in Table 4.6 where the $R^2$ for ICC Elongation is -1.25. A negative $R^2$ is mathematically possible and usually occurs when $SS_{err}$ is larger than $SS_{tot}$ as is the case here. This indicates that the fit between the ICC and manually measured Elongation is very poor. Similarly, the $R^2$ for ICC Flatness is less than 0.60 implying that a straight-line/linear model cannot be used to relate the ICC Flatness to manually measured Flatness (Mendenhall & Sincich 2006). It is noted that, in terms of Equancy (S/L), ICC is by far the strongest performer. This can be explained by its ability to approximate ‘L’ and ‘S’ with greater accuracy.

Equancy is not an independent Form ratio, but is a product of Elongation and Flatness. Furthermore, both Flatness and Elongation are dependent on the intermediate diameter ‘I’. It is therefore reasonable to conclude that the intermediate diameter is the fundamental parameter that should be used when comparing different methods of Form measurement.

Based on this, it is clear that GBE is the better method for approximating dimensions (for ballast particles) since it has the greatest accuracy when approximating ‘I’. This translates in turn to the best linear fit of all the Form ratios against manually measured ratios.
Figure 4.26 Comparison of Inscribed and circumscribed circle diameter (ICC) vs. Manual measurements

Figure 4.27 Comparison of equivalent inertia ellipse diameters (EIE) vs. Manual measurements
Figure 4.28 Comparison of geometric best-fit ellipse diameter (GBE) vs. Manual measurements

Figure 4.29 Comparison of Form ratios using Inscribed and circumscribed circle diameter (ICC) vs manual measurements
Figure 4.30 Comparison of Form ratios using Equivalent inertia ellipse diameters (EIE) vs manual measurements

Figure 4.31 Comparison of Form ratios using geometric best-fit ellipse diameter (GBE) vs manual measurements
4.4.2. Cliffe Hill specimen

The diameters (S, I and L) for individual particles in the specimen described in Section 4.3.1 and their shape characterisation analysis are presented here.

Table 4.7 gives a statistical description of the estimated diameters for the specimen while the boxplot in Figure 4.32 provides a graphical overview of the observations that have been made.

It is clear from Figure 4.32 that the longest diameter L has a greater variation and spread than both I and S. This is confirmed by its standard deviation (SD) and inter-quartile range (IQR) (Table 4.7 and Table 4.8). The longest diameter has a standard deviation 59% and 38% greater than S and I respectively. Its IQR (in Table 4.8) is 47% and 40% larger. This is most likely a consequence of the mineralogy and morphology of the aggregate.

The outliers in Figure 4.32, denoted by crosses beyond the whiskers, are most likely erroneous readings caused by image processing artefacts. The mean and median for the different diameters are essentially similar, suggesting that there is minimal skew from a normal distribution. This is illustrated in Figure 4.33–Figure 4.35.

Figure 4.36 shows the result of a virtual PSD analysis that was carried out using the dimensions acquired from image analysis. It is important to note that since the PSD analysis of the ballast material (as described in section 3.3.1) was carried out on the basis of mass, the virtual sieving should also be based on mass to make any comparison meaningful. To achieve this, the mass of each of the particles was calculated using the volume of the equivalent ellipsoid (from S, I and L) and a material density of 2650kg/m³. The imaged ballast particles were separated (or “virtually sieved”) based on their cross-sectional area (calculated from S and I) relative to the different sieve size aperture cross-sectional areas. Finally, the masses retained and passing were calculated for each sieve size. Figure 4.36 shows that the specimen has a representative PSD.
4. Dev. and characterisation of DEM railway ballast

Table 4.7 Descriptive statistics for the S I and L for Cliffe Hill ballast

<table>
<thead>
<tr>
<th></th>
<th>Range</th>
<th>Minimum</th>
<th>Maximum</th>
<th>Mean</th>
<th>Median</th>
<th>Std. Dev.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Smallest  (S)</td>
<td>52.52</td>
<td>16.86</td>
<td>69.37</td>
<td>42.34</td>
<td>43.85</td>
<td>12.38</td>
</tr>
<tr>
<td>Intermediate (I)</td>
<td>93.59</td>
<td>27.22</td>
<td>120.81</td>
<td>69.34</td>
<td>69.53</td>
<td>18.62</td>
</tr>
<tr>
<td>Largest (L)</td>
<td>129.19</td>
<td>44.08</td>
<td>173.26</td>
<td>101.28</td>
<td>102.83</td>
<td>30.27</td>
</tr>
</tbody>
</table>

Table 4.8 Percentile and IQR data for the S I and L for Cliffe Hill ballast

<table>
<thead>
<tr>
<th></th>
<th>25th</th>
<th>50th</th>
<th>75th</th>
<th>IQR</th>
</tr>
</thead>
<tbody>
<tr>
<td>S</td>
<td>32.04</td>
<td>43.85</td>
<td>51.96</td>
<td>19.93</td>
</tr>
<tr>
<td>I</td>
<td>57.15</td>
<td>69.53</td>
<td>79.76</td>
<td>22.61</td>
</tr>
<tr>
<td>L</td>
<td>79.90</td>
<td>102.83</td>
<td>117.32</td>
<td>37.41</td>
</tr>
</tbody>
</table>

Figure 4.32 Boxplot of S I and L diameters for Cliffe Hill. The box represents part of the specimen enclosed by the 25th and 75th percentile and the median diameter is shown by the horizontal line within the box. The whiskers show the lowest and highest measurement still within ±1.5×IQR. Outliers are shown by plus signs.
Figure 4.33 Histogram showing the distribution of the Smallest diameter for the Cliffe Hill ballast

Figure 4.34 Histogram showing the distribution of the Intermediate diameter for the Cliffe Hill ballast
Figure 4.35 Histogram showing the distribution of the Largest diameter for the Cliffe Hill ballast

Figure 4.36 PSD analysis of using image based measurements for the Cliffe Hill ballast
The Form characteristics of the Cliffe Hill specimen were analysed using the parameters stated in Section 4.3.5. Table 4.9 and Table 4.10 present the descriptive statistics for the specimen. A graphical representation is given in Figure 4.37.

The median Elongation and Flatness are 0.715 and 0.608 respectively. This suggests that, on average, the particles in the specimen are moderately flat and elongated based on the classification in Table 4.11 proposed by Blott and Pye (2008). Similarly the 25th and 75th percentile values for elongation and flatness suggest that the specimen, as a whole, ranges from ‘Slightly – Not elongate’ and ‘Moderately – Slightly flat’. The maximum and minimum are not used as they represent the extremes of the dataset.

From the Zingg diagram (Figure 4.39), it can be seen that the majority of the particles can be classified as being either flat (42%) or spherical (38%) in 3D Form. Using a data clustering technique (based on distances) it can be seen that 71% of I/L lie between 0.566 to 0.936 and S/I lie between 0.401 to 0.771. This is indicated in Figure 4.39 by the dashed line.

Figure 4.40 is a modified Zingg diagram (after Blott and Pye (2008)) that includes contours of Equancy ratio. As a whole, 86% of the specimen can be considered as ‘Very – Moderately non-equant’.

Ellipseness is used here as a measure of particle angularity. 84% of the specimen has as Ellipseness value ranging between 0.8 and 0.9; the average Ellipseness of the specimen is 0.85. As shown in Figure 4.41, the distribution of Ellipseness is highly concentrated about the median with a very low standard deviation. This is not unexpected since the particles are all from the same parent rock. While Form can be largely dependent on the manufacturing process (e.g. the type of crusher), angularity is reliant on the mineralogy of the rock and its crystalline structure which can influence how cracks propagate.
### Table 4.9 Descriptive statistics for the Form parameters for Cliffe Hill ballast

<table>
<thead>
<tr>
<th></th>
<th>Range</th>
<th>Min</th>
<th>Max</th>
<th>Mean</th>
<th>Median</th>
<th>Std. Dev.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elongation (I/L)</td>
<td>0.56</td>
<td>0.39</td>
<td>0.94</td>
<td>0.703</td>
<td>0.715</td>
<td>0.128</td>
</tr>
<tr>
<td>Flatness (S/I)</td>
<td>0.69</td>
<td>0.29</td>
<td>0.98</td>
<td>0.623</td>
<td>0.608</td>
<td>0.145</td>
</tr>
<tr>
<td>Equancy (S/L)</td>
<td>0.70</td>
<td>0.20</td>
<td>0.90</td>
<td>0.435</td>
<td>0.422</td>
<td>0.126</td>
</tr>
</tbody>
</table>

### Table 4.10 Percentile and IQR data for the Form parameters Cliffe Hill ballast

<table>
<thead>
<tr>
<th></th>
<th>25th</th>
<th>50th</th>
<th>75th</th>
<th>IQR</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elongation (I/L)</td>
<td>0.625</td>
<td>0.715</td>
<td>0.812</td>
<td>0.19</td>
</tr>
<tr>
<td>Flatness (S/I)</td>
<td>0.514</td>
<td>0.609</td>
<td>0.728</td>
<td>0.21</td>
</tr>
<tr>
<td>Equancy (S/L)</td>
<td>0.333</td>
<td>0.422</td>
<td>0.513</td>
<td>0.18</td>
</tr>
</tbody>
</table>

### Table 4.11 Classification terminology for particle form, based on the degree of elongation (I/L), flatness (S/I) and Equancy (S/L) (Blott & Pye 2008).

<table>
<thead>
<tr>
<th>Elongation</th>
<th>Flatness</th>
<th>Equancy</th>
</tr>
</thead>
<tbody>
<tr>
<td>I/L</td>
<td>Term</td>
<td>S/I</td>
</tr>
<tr>
<td>0.0 – 0.2</td>
<td>Extremely elongate</td>
<td>0.0 – 0.2</td>
</tr>
<tr>
<td>0.2 – 0.4</td>
<td>Very elongate</td>
<td>0.2 – 0.4</td>
</tr>
<tr>
<td>0.4 – 0.6</td>
<td>Moderately elongate</td>
<td>0.4 – 0.6</td>
</tr>
<tr>
<td>0.6 – 0.8</td>
<td>Slightly elongate</td>
<td>0.6 – 0.8</td>
</tr>
<tr>
<td>0.8 – 1.0</td>
<td>Not Elongate</td>
<td>0.8 – 1.0</td>
</tr>
</tbody>
</table>
4. Dev. and characterisation of DEM railway ballast

Figure 4.37 Boxplot of Form parameters for Cliffe Hill

Figure 4.38 Visual key for Znigg plot (Blott & Pye 2008)
Figure 4.39 Zingg’s bivariate diagram of Elongation and Flatness for Cliffe Hill

Figure 4.40 Modified Zingg diagram to include Equancy.
Table 4.12 Descriptive statistics of Ellipseness for Cliffe Hill

<table>
<thead>
<tr>
<th>Statistic</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>0.8476</td>
</tr>
<tr>
<td>Median</td>
<td>0.8588</td>
</tr>
<tr>
<td>Std. Deviation</td>
<td>0.0419</td>
</tr>
<tr>
<td>IQR</td>
<td>0.0405</td>
</tr>
<tr>
<td>Range</td>
<td>0.3031</td>
</tr>
<tr>
<td>Minimum</td>
<td>0.5961</td>
</tr>
<tr>
<td>Maximum</td>
<td>0.8992</td>
</tr>
<tr>
<td>25th Percentile</td>
<td>0.8331</td>
</tr>
<tr>
<td>50th Percentile</td>
<td>0.8588</td>
</tr>
<tr>
<td>75th Percentile</td>
<td>0.8736</td>
</tr>
</tbody>
</table>

Figure 4.41 Histogram showing the distribution Ellipseness of Cliffe Hill ballast. The two photos represents a typical partial with the associated Ellipseness.
4.4.3. Comparison of Cliffe Hill to Glensanda ballast

To gain a better understanding of the extent to which particle shape may vary among different types of ballast, the Cliffe Hill (CH) ballast is compared to a specimen of ballast sourced from the Glensanda (GS) quarry (on the Morvern peninsula in the western Highlands) operated by Aggregate Industries. It meets the same specification (BS EN 13450:2002 grading category A) as CH in terms of PSD. Unlike the Cliffe hill specimen (granodiorite), the Glensanda material is of the Granite type in the Igneous group. The ballast from Glensanda was similarly prepared to the Cliffe Hill one and put through the same image acquisition and analysis methods.

Figure 4.43 compares the Elongation (I/L) ratio of the two specimens. The two boxplots look very similar. However, the IQR and standard deviation (in Table 4.13) indicate that the CH specimen has a wider variation in elongation. Further, a comparison of the median shows that, on average, GS ballast particles are 4.74% less elongated than CH ballast particles. The difference between the specimens becomes more pronounced when the Flatness ratio is compared (Figure 4.44 and Table 4.14). The median S/I for CH and GS are 0.609 and 0.740 respectively. This means that the CH specimen is 17.7% flatter.

To appreciate fully these differences in Form, the Zingg diagrams of the specimens are compared. Figure 4.46 shows that there are 37% more particles that can be classed as ‘spherical’ in Form in the GS specimen, and 31% fewer flat particles, than in CH.

A similar trend is seen in the S/L ratio for GS ballast. 88% of the particles can be classified as ‘Slightly – Moderately non-equant’. Conversely, 86% of the CH ballast is classed as ‘Very – Moderately non-equant’ (Figure 4.47).

This quantifiable difference in Form between the two types of ballast can be explained by considering their different petrology. While both specimens are of igneous rocks, granite differs from granodiorite in that at least 35% of the feldspar (tectosilicate minerals) in granite is alkali feldspar as opposed to plagioclase (Klein & Dutrow 2008). The presence of alkali feldspar is what gives (much) granite its distinctive pink colour as is apparent in Figure 4.42. As well as the mineralogical
differences, there will also be variations in crystal grain size, orientation of crystals and porosity (Brewer 1964).

\[ \text{Figure 4.42 Ballast from Glensanda (left) and Cliffe hill (right).} \]

As a consequence, cracks will propagate differently during crushing which in turn results in dissimilar Form in the resulting ballast.

As the specimens are produced by two different companies, the manufacturing process may also be different. There are a variety of rock crushers (e.g. jaw, cone, impact) and automatic sieves (e.g. circular, square) that can be employed in any combination by producers. It is therefore reasonable to conclude that this will also have an effect on particle Form.

For the above reasons differences in angularity may also be expected between CH and GS. Figure 4.48 compares their Ellipseness (E). On average, GS ballast is 3.6% more elliptic than CH. Furthermore, ballast from CH has a 55% greater range of variably of Ellipseness, as shown by comparing the IQR’s.

In general, the comparison shows that even though material from Cliffe Hill and Glensanda meet current Network Rail specification for crushed rocks as ballast they are measurably different in shape especially in terms of flatness.
Figure 4.43 Comparison of Elongation (I/L) for Cliffe Hill and Glensanda

Table 4.13 Descriptive statistics of Elongation (I/L) for Cliffe Hill and Glensanda

<table>
<thead>
<tr>
<th></th>
<th>Cliffe Hill</th>
<th>Glensanda</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>0.703</td>
<td>0.732</td>
</tr>
<tr>
<td>Median</td>
<td>0.716</td>
<td>0.750</td>
</tr>
<tr>
<td>Std. Deviation</td>
<td>0.129</td>
<td>0.120</td>
</tr>
<tr>
<td>IQR</td>
<td>0.188</td>
<td>0.167</td>
</tr>
<tr>
<td>Range</td>
<td>0.555</td>
<td>0.569</td>
</tr>
<tr>
<td>Minimum</td>
<td>0.388</td>
<td>0.391</td>
</tr>
<tr>
<td>Maximum</td>
<td>0.943</td>
<td>0.960</td>
</tr>
<tr>
<td>Percentiles</td>
<td></td>
<td></td>
</tr>
<tr>
<td>25th</td>
<td>0.625</td>
<td>0.646</td>
</tr>
<tr>
<td>50th</td>
<td>0.716</td>
<td>0.750</td>
</tr>
<tr>
<td>75th</td>
<td>0.812</td>
<td>0.813</td>
</tr>
</tbody>
</table>
Figure 4.44 Comparison Flatness (S/I) for Cliffe Hill and Glensanda

Table 4.14 Descriptive statistics of Flatness (S/I) for Cliffe Hill and Glensanda

<table>
<thead>
<tr>
<th></th>
<th>Cliffe Hill</th>
<th>Glensanda</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>0.623</td>
<td>0.746</td>
</tr>
<tr>
<td>Median</td>
<td>0.609</td>
<td>0.740</td>
</tr>
<tr>
<td>Std. Deviation</td>
<td>0.146</td>
<td>0.143</td>
</tr>
<tr>
<td>IQR</td>
<td>0.214</td>
<td>0.216</td>
</tr>
<tr>
<td>Range</td>
<td>0.686</td>
<td>0.547</td>
</tr>
<tr>
<td>Minimum</td>
<td>0.293</td>
<td>0.448</td>
</tr>
<tr>
<td>Maximum</td>
<td>0.979</td>
<td>0.995</td>
</tr>
<tr>
<td>Percentiles</td>
<td></td>
<td></td>
</tr>
<tr>
<td>25th</td>
<td>0.514</td>
<td>0.642</td>
</tr>
<tr>
<td>50th</td>
<td>0.609</td>
<td>0.740</td>
</tr>
<tr>
<td>75th</td>
<td>0.728</td>
<td>0.858</td>
</tr>
</tbody>
</table>
Figure 4.45 Comparison Equancy (S/L) for Cliffie Hill and Glensanda

Table 4.15 Descriptive statistics of Equancy (S/L) for Cliffie Hill and Glensanda

<table>
<thead>
<tr>
<th></th>
<th>Cliffie Hill</th>
<th>Glensanda</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>0.435</td>
<td>0.542</td>
</tr>
<tr>
<td>Median</td>
<td>0.422</td>
<td>0.551</td>
</tr>
<tr>
<td>Std. Deviation</td>
<td>0.126</td>
<td>0.117</td>
</tr>
<tr>
<td>IQR</td>
<td>0.180</td>
<td>0.167</td>
</tr>
<tr>
<td>Range</td>
<td>0.700</td>
<td>0.541</td>
</tr>
<tr>
<td>Minimum</td>
<td>0.200</td>
<td>0.318</td>
</tr>
<tr>
<td>Maximum</td>
<td>0.899</td>
<td>0.858</td>
</tr>
<tr>
<td>25th Percentiles</td>
<td>0.333</td>
<td>0.450</td>
</tr>
<tr>
<td>50th Percentiles</td>
<td>0.422</td>
<td>0.551</td>
</tr>
<tr>
<td>75th Percentiles</td>
<td>0.513</td>
<td>0.617</td>
</tr>
</tbody>
</table>
Figure 4.46 Zingg’s bivariate diagram of Elongation and Flatness for Glensanda

Figure 4.47 Modified Zingg diagram to include Equancy.
Figure 4.48 Comparison of Ellipsenness between Cliffe Hill and Glensanda ballast

<table>
<thead>
<tr>
<th></th>
<th>Cliffe Hill</th>
<th>Glensanda</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>0.848</td>
<td>0.888</td>
</tr>
<tr>
<td>Median</td>
<td>0.859</td>
<td>0.890</td>
</tr>
<tr>
<td>Std. Deviation</td>
<td>0.042</td>
<td>0.016</td>
</tr>
<tr>
<td>IQR</td>
<td>0.040</td>
<td>0.018</td>
</tr>
<tr>
<td>Range</td>
<td>0.303</td>
<td>0.073</td>
</tr>
<tr>
<td>Minimum</td>
<td>0.596</td>
<td>0.841</td>
</tr>
<tr>
<td>Maximum</td>
<td>0.899</td>
<td>0.914</td>
</tr>
<tr>
<td>Percentiles</td>
<td></td>
<td></td>
</tr>
<tr>
<td>25th</td>
<td>0.833</td>
<td>0.881</td>
</tr>
<tr>
<td>50th</td>
<td>0.859</td>
<td>0.890</td>
</tr>
<tr>
<td>75th</td>
<td>0.874</td>
<td>0.898</td>
</tr>
</tbody>
</table>
4.5. Development and characterisation of DEM ballast

The DEM ballast particles were constructed on the basis of the appearance of individual ballast particles picked at random from the Cliffe Hill specimen [consisting of 100 particles] characterised previously. The computer program utilised for this process is a further development by Harkness (2009) to the concept of Potential Particles and further described in Ahmed et al (2014).

A basic sphere of unit radius, as shown in Figure 4.49, was used as the starting point for each particle. The Red, Green and Blue spots represent points on the X, Y and Z axes of the sphere. A number of flat surfaces (or ‘flats’) are then added to the sphere to recreate the shape of the particular ballast particle being modelled. Each of the flats has a control node (the dark blue sphere in Figure 4.50) which allows the flat to be moved around the sphere in 3D space. The area of the flats can be increased or decreased by pushing the flat surface into, or pulling it out of, the sphere using the control node.

A minimum of four flats can be used to construct a DEM ballast particle, resulting in a tetrahedral particle. However, real ballast particles have, on average, 7 faces that make up the surface envelope (Meloy & Ahluwalia 2002). Using the control nodes, each of the flats is placed into an arrangement similar to the ballast particle being constructed.

Figure 4.51 shows how flats are incrementally added to create a DEM ballast particle of arbitrary shape and Figure 4.52 shows a comparison between a real ballast particle and its DEM representation. In total fourteen DEM ballast particles were constructed using the process described above. Images of three orthogonal views for each of the particles were generated and saved. An example of this is shown in Figure 4.53: a base sphere is also included in each of the images as a scale reference for spatial calibration during image analysis. The resolution of the images was set to 300dpi, in line with the images of the Cliffe hill specimen. The images are then analysed as before.
Figure 4.49 The sphere is the base particle

Figure 4.50 3D drawing showing the control node and its degrees of freedom

Figure 4.51 From a sphere to an arbitrary shaped particle
Figure 4.52 Example numerical ballast particle with its real counterpart

Figure 4.53 Three orthogonal views of a DEM ballast
4.5.1. Comparison of DEM ballast with Cliffe hill specimen.

Figure 4.54 shows a comparison of particle Elongation for the Cliffe Hill ballast (CH) and DEM ballast (DB). The average elongation ratio for the DB is 6.28% smaller than for CH indicating that the DB is only slightly more elongated. There is also a marginally larger variation in elongation with the DB as seen with the standard deviation and IQR in (Table 4.17). Overall, the boxplot and comparative statistics suggest that the DB captures very well the elongation characteristics of real ballast.

Although the median Flatness of DB only varies by 4.43% from CH, the IQR, which is almost twice as large as for CH, indicating that there is very high dispersion (Figure 4.55). This can be attributed to the method used to construct the DEM ballast. Even though the particle designer module works in 3D space, the operator can only see a 2D rendition through the computer monitor. As a consequence there is a distorted perception of depth resulting in particles that can vary widely in Flatness. In spite of this, the overall range of the flatness ratio for DB is comparable with CH, as are the maximum and minimum values. This can be seen in Table 4.18. Thus the DB captures the flatness of CH reasonably well.

Table 4.19 and Figure 4.56 show the comparative statistics and their graphical representation for the Equancy ratio. As with the Elongation ratio, there is very good correlation between the DB and CH in terms of Equancy. This is also seen in Figure 4.58 where 85.7% of the DEM particles are classified as ‘Very – Moderately non-equant’ compared to 86% of CH with the same classification.

Ellipseness is different for the Cliffe Hill and DEM ballast. This is evident in Figure 4.59, where there is no overlap between the boxes for DB and CH. DB ballast particles are slightly more elliptical than the Cliffe hill specimen. What is perhaps more interesting is that while the IQR for both specimens are exactly the same, the standard deviation for CH is at least double that of DB. The greater variances in CH are a direct result of natural variation seen in crushed rocks. Conversely, the minimal variation for the DEM ballast is due to its origin as a mathematical construct.
The results shown in Table 4.20 and Figure 4.59 were not unexpected. Given the geometric properties of potential particles, the surfaces that make up the particle are defined as ‘strictly convex’ (i.e. not completely flat). While the curvature of the strictly convex surface can be controlled, contact detection can become unreliable as the surfaces tends towards perfectly flat contributing to numerical instability. For this reason DEM particles are inherently more “rounded” than the actual particles they are meant to represent.
4. Dev. and characterisation of DEM railway ballast

![Comparison of Elongation for Cliffe hill and DEM ballast](image)

**Figure 4.54** Comparison of Elongation for Cliffe hill and DEM ballast

**Table 4.17** Descriptive statistics of Elongation (I/L) for Cliffe Hill DEM ballast

<table>
<thead>
<tr>
<th>Statistic</th>
<th>Cliffe Hill</th>
<th>DEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>0.703</td>
<td>0.667</td>
</tr>
<tr>
<td>Median</td>
<td>0.716</td>
<td>0.671</td>
</tr>
<tr>
<td>Std. Deviation</td>
<td>0.129</td>
<td>0.140</td>
</tr>
<tr>
<td>IQR</td>
<td>0.188</td>
<td>0.209</td>
</tr>
<tr>
<td>Range</td>
<td>0.555</td>
<td>0.523</td>
</tr>
<tr>
<td>Minimum</td>
<td>0.388</td>
<td>0.381</td>
</tr>
<tr>
<td>Maximum</td>
<td>0.943</td>
<td>0.904</td>
</tr>
<tr>
<td>25th Percentile</td>
<td>0.625</td>
<td>0.564</td>
</tr>
<tr>
<td>50th Percentile</td>
<td>0.716</td>
<td>0.671</td>
</tr>
<tr>
<td>75th Percentile</td>
<td>0.812</td>
<td>0.773</td>
</tr>
</tbody>
</table>
Figure 4.55 Comparison of Flatness for Cliffe hill and DEM ballast

Table 4.18 Descriptive statistics of Flatness (S/I) for Cliffe Hill DEM ballast

<table>
<thead>
<tr>
<th></th>
<th>Cliffe Hill</th>
<th>DEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>0.623</td>
<td>0.651</td>
</tr>
<tr>
<td>Median</td>
<td>0.609</td>
<td>0.636</td>
</tr>
<tr>
<td>Std. Deviation</td>
<td>0.146</td>
<td>0.214</td>
</tr>
<tr>
<td>IQR</td>
<td>0.214</td>
<td>0.420</td>
</tr>
<tr>
<td>Range</td>
<td>0.686</td>
<td>0.638</td>
</tr>
<tr>
<td>Minimum</td>
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<td>0.339</td>
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<td>Maximum</td>
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<td>0.976</td>
</tr>
<tr>
<td>Percentiles</td>
<td></td>
<td></td>
</tr>
<tr>
<td>25th</td>
<td>0.514</td>
<td>0.436</td>
</tr>
<tr>
<td>50th</td>
<td>0.609</td>
<td>0.636</td>
</tr>
<tr>
<td>75th</td>
<td>0.728</td>
<td>0.856</td>
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</tbody>
</table>
Figure 4.56 Comparison of Equancy for Cliffe hill and DEM ballast

Table 4.19 Descriptive statistics of Equancy (S/L) for Cliffe Hill DEM ballast

<table>
<thead>
<tr>
<th></th>
<th>Cliffe Hill</th>
<th>DEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>0.435</td>
<td>0.419</td>
</tr>
<tr>
<td>Median</td>
<td>0.422</td>
<td>0.413</td>
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<tr>
<td>Std. Deviation</td>
<td>0.126</td>
<td>0.126</td>
</tr>
<tr>
<td>IQR</td>
<td>0.180</td>
<td>0.164</td>
</tr>
<tr>
<td>Range</td>
<td>0.700</td>
<td>0.441</td>
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<tr>
<td>Minimum</td>
<td>0.200</td>
<td>0.215</td>
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<td>0.899</td>
<td>0.656</td>
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<td>25&lt;sup&gt;th&lt;/sup&gt;</td>
<td>0.333</td>
<td>0.331</td>
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<tr>
<td>50&lt;sup&gt;th&lt;/sup&gt;</td>
<td>0.422</td>
<td>0.413</td>
</tr>
<tr>
<td>75&lt;sup&gt;th&lt;/sup&gt;</td>
<td>0.513</td>
<td>0.495</td>
</tr>
</tbody>
</table>
Figure 4.57 Zingg’s bivariate diagram of Elongation and Flatness for DEM ballast

Figure 4.58 Modified Zingg diagram to include Equancy.
Figure 4.59 Comparison of Ellipseness for Cliffe hill and DEM ballast

Table 4.20 Descriptive statistics of Ellipseness for Cliffe Hill DEM ballast

<table>
<thead>
<tr>
<th></th>
<th>Cliffe Hill</th>
<th>DEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>0.848</td>
<td>0.896</td>
</tr>
<tr>
<td>Median</td>
<td>0.859</td>
<td>0.894</td>
</tr>
<tr>
<td>Std. Deviation</td>
<td>0.042</td>
<td>0.023</td>
</tr>
<tr>
<td>IQR</td>
<td>0.040</td>
<td>0.040</td>
</tr>
<tr>
<td>Range</td>
<td>0.303</td>
<td>0.077</td>
</tr>
<tr>
<td>Minimum</td>
<td>0.596</td>
<td>0.849</td>
</tr>
<tr>
<td>Maximum</td>
<td>0.899</td>
<td>0.926</td>
</tr>
<tr>
<td>Percentiles 25th</td>
<td>0.833</td>
<td>0.879</td>
</tr>
<tr>
<td>50th</td>
<td>0.859</td>
<td>0.894</td>
</tr>
<tr>
<td>75th</td>
<td>0.874</td>
<td>0.918</td>
</tr>
</tbody>
</table>
4.6. Summary

Given the sharp drop in prices of computing and imaging equipment in the past 10 years, it is not surprising to find great diversity in how workers in the field have implemented image data acquisition for particle characterisation. It is evident from the literature that dynamic imaging systems are perhaps the most popular ones due mainly to their high output rates. Systems such as the University of Illinois Aggregate Image Analyser (UIAIA) are expensive with a capital estimated cost of $35,000 (Rousan 2004). A substantial portion of this cost will have gone into the particle transport mechanism and its automation. A practical alternative based on static imaging is proposed here at 1/10th of the cost of the UIAIA, with an output rate of 300 particles per hour.

Following image capture, thresholding is perhaps the most critical stage of the post-processing phase. The use of a green background, in conjunction with a colour based segmentation implemented here, has been shown to provide a robust method of distinguishing the particle from the background.

The proposed geometric best-fit ellipse (GBE) can be computationally intensive given that it is an iterative method. However the use of parallelisation tools (e.g. Matlab’s parfor) in conjunction with multi-core personal computing reduced computation time significantly making GBE algorithm feasible.

Comparison between the different image based diameter measurement methods and the manual method showed GBE to be the most robust and reliable justifying the additional computational effort.

Comparison between two sources of ballast showed that they have quite different shapes, even though they meet the same Network Rail specification. It is logical to conclude that the variation in shape is as a result of the differences in mineralogy and manufacturing processes.

Finally, the numerical DEM ballast was modelled to capture, as best as possible, the shape characteristics of the natural ballast sourced from Cliffe Hill quarry.
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5

Modelling of triaxial testing on ballast

5.1. Introduction

The triaxial shear test is a common and perhaps the most widely used laboratory element test for determining strength and stiffness parameters of a soil. However, it can be difficult to carry out representative mechanical testing on specimens of railway ballast in this type of laboratory apparatus owing to the large particle size. Even in situations where large scale element tests are possible, it remains very difficult to monitor and analyse the particle scale mechanisms that underlie the complex overall material response that takes place during loading. This makes it difficult to unpick the influence different particle shape parameters have on the fabric that develops and the consequent material response. Although Chapter 3 has shown that X-ray CT can be used to overcome has for at least one instant in time (where the tested specimen is ‘frozen’ in time with resin), real time monitoring and probing of data such as particle orientation during testing remains extremely challenging.

Fortunately, numerical modelling using the Discrete Element Method (DEM) provides a means to overcome this barrier allowing the evaluation of particle scale variables such as the individual contact forces, the particle and contact orientations, etc. Its use has greatly advanced the understanding of soil behaviour at a particulate scale (e.g., Thornton 2000; McDowell & de Bono 2013). However,
a point of contention remains with regard to the choice of particle shape and its importance to the behaviour of granular media (e.g., Lu & McDowell 2007).

In this chapter a new DEM model of the triaxial cell test is developed using numerical ballast particles, incorporating the shape information of real ballast, which has been established in the previous chapter. The computer program utilised for this process is a further development by Harkness (2009) to the concept of Potential Particles and further described in Ahmed et al (2014).

This chapter:-

- describes the simulation of a triaxial test, including specimen preparation and the application of a confining pressure.
- presents an investigation into the effects of variations in physical and modelling parameters on the test results and identifies values that match the laboratory behaviour.
- presents insights into the fabric of ballast gained from a DEM simulation of a triaxial test that matches volumetric and strength behaviour to that observed in a physical test.
5.2. A brief overview of the discrete element method.

A discrete element method (DEM) is any of a family of numerical methods for computing or simulating the finite displacements and rotations of a number of interacting discrete bodies. These methods are able to analyse multiple interacting bodies undergoing large dynamic movements making them well suited to solving problems that exhibit gross discontinuous behaviour.

There are two categories of DEM that are most commonly used; the soft sphere model and hard sphere model (Zhu et al. 2007; Luding 2008).

In the soft sphere approach, particles that come into contact are allowed to overlap or penetrate each other by a small amount. Figure 5.1A shows the overlap that occurs at the contact of two particles. These overlaps are then used to calculate the elastic, plastic and frictional forces at the contacts.

![Figure 5.1](image1.png)

*Figure 5.1 (A) Contact between two ‘soft sphere’ particles and (B) Contact between two ‘hard sphere’ particles*

![Figure 5.2](image2.png)

*Figure 5.2 a simple potential particle (Houlsby 2009).*
The rotational and translational motion of the particles is governed by Newton’s laws of motion. Perhaps the most characteristic feature of this approach is its ability to handle multiple simultaneous contacts. This allows the modelling of static/quasi-static problems that typically arise in soil mechanics. The seminal publication in this area is considered to be the one by Cundall and Strack (1979).

It should be noted that particles in the soft sphere approach are in fact rigid and unable to physically deform. However, real particles tend to deform at the contacts and the overlap provides a simple and effective means of modelling this deformation.

The hard sphere approach, on the other hand, does not allow interpenetration or overlap (Figure 5.1B). Furthermore, collision events are analysed sequentially one collision at a time (Zhu et al. 2007). As a result, the hard sphere method is well suited for rapid granular flow problems (such as avalanches) where granular matter has been fluidized.

The soft sphere approach has been used for the work presented here.

5.2.1. Particle geometry

Particle geometry (i.e. shape) has a significant influence on the mechanical behaviour of granular media such as sands and aggregates. Since natural particles are arbitrary in shape, it is important that the geometries used in DEM modelling are representative of the material being simulated. While there are many established methods for generating arbitrary shaped particles, not all are viable because of the associated contact detection algorithms being highly complex and computationally expensive.

Houlsby (2009) proposed an approach whereby 2D non-circular particles are defined by some (smooth) function in a local coordinate system. Using a local coordinate vector \( \mathbf{X} \), such a ‘Potential Particle’ can be described by a function \( f(\mathbf{X}) \) such that,

\[
\begin{align*}
  f(\mathbf{X}) & \begin{cases} 
    < 0 & \text{inside the particle} \\
    = 0 & \text{on the particle surface} \\
    > 0 & \text{outside the particle}
  \end{cases}
\end{align*}
\]  \hspace{1cm} (4.1)
To simplify contact detection, multiple contacts between particle pairs are eliminated by specifying that any surface defined by \( f(\mathbf{X}) = \text{constant} \) must be strictly convex. A simple elliptic particle defined in this way is illustrated in Figure 5.2. The shaded area represents the particle, and the lines are contours of \( f(\mathbf{X}) = \text{constant} \).

The state of contact between two such particles, \( P_1 \) and \( P_2 \), (defined by \( f_1(\mathbf{X}) \) and \( f_2(\mathbf{X}) \)) can be determined by minimising \( f_2 \) subject to the constraint \( f_1(\mathbf{X}) = 0 \) such that:

\[
f_2(\mathbf{X}) + \Lambda f_1(\mathbf{X}) = 0
\]

where \( \Lambda \) is a Lagrangian multiplier used for the minimisation. It follows that:

\[
\nabla f_2(\mathbf{X}) = -\Lambda \nabla f_1(\mathbf{X})
\]

The Lagrangian multiplier can be eliminated from the pair of simultaneous equations given by Equation 4.3. A non-linear solver (e.g. Newton-Raphson) can then be used to solve for \( \mathbf{X} \). So, if \( f_2(\mathbf{X}) > 0 \) then no contact exists (Figure 5.3A), if \( f_2(\mathbf{X}) = 0 \) then \( P_1 \) and \( P_2 \) are just touching (Figure 5.3B), while if \( f_2(\mathbf{X}) < 0 \) then the particles are overlapping as shown in Figure 5.3C. This is a very rudimentary description and the interested reader is directed to the original work by Houlsby (2009) for a detailed discussion.

Using this concept, simple shapes such as circles and ellipses can be defined using potentials of the form:

\[
f = x^2 + y^2 - r^2 \quad \text{a circle of radius } r
\]

\[
f = \frac{x^2}{a^2} + \frac{y^2}{b^2} - 1 \quad \text{an ellipse with axes } a \text{ and } b
\]

Further, more complex shapes can also be built by assembling a number of potential functions of lines in 2D. A 3D generalisation, using surfaces, has been developed by Harkness (2009). The corresponding 2D/3D potential function is of the form,

\[
f(x,y,z) = (1 - k) \left( \sum_{i=1}^{n} (a_i x + b_i y + c_i z + d_i)^2 - r^2 \right) + k (x^2 + y^2 + z^2 - R^2)
\]
where $0 < k < 1$ defines the curvature of the faces (lines or surfaces), $r$ is a constant and related to the curvature of the corners where two lines/surfaces meet. The McCauley brackets $\langle \cdot \rangle$ define a function such that $\langle x \rangle = x$ if $x > 0$ and $\langle x \rangle = 0$ when $x \leq 0$.

![Figure 5.3 Two potential particles A: not in contact B: just touching C: in contact with overlap](image)

Figure 5.3 Two potential particles A: not in contact B: just touching C: in contact with overlap

![Figure 5.4 Potential function development. A: triangle composed of three lines B: triangle defined by Potential function (Harkness 2009)](image)

Figure 5.4 Potential function development. A: triangle composed of three lines B: triangle defined by Potential function (Harkness 2009)

Figure 5.4A shows how three lines; $y + \frac{1}{\sqrt{3}} = 0$, $y + \sqrt{3}x - \frac{2}{\sqrt{3}} = 0$ and $y - \sqrt{3}x - \frac{2}{\sqrt{3}} = 0$ can be used to define a triangle that is strictly convex. The potential function describing the particle in Figure 5.4B is then,

\[
f(x, y) = (1 - k) \left\{ -y - \frac{1}{\sqrt{3}} \right\}^2 + \left\{ y + \sqrt{3}x - \frac{2}{\sqrt{3}} \right\}^2 + \left\{ y - \sqrt{3}x - \frac{1}{\sqrt{3}} \right\}^2
- r \right\} + k \left\{ x^2 + y^2 - \left( \frac{2}{\sqrt{3}} \right)^2 \right\}
\]

(4.6)
where \( r = 0.1 \) and \( k = 0.01 \). While the rounded triangle in Figure 5.4B appears to have straight sides, they are in fact slightly curved. A detailed explanation of this example can be found in Harkness (2009).

\[
\begin{align*}
\mathbf{r}_x &= k_r \mathbf{r}_x^{desired} \\
\mathbf{r}_y &= k_r \mathbf{r}_y^{desired}
\end{align*}
\]

\( (4.8) \)

**Figure 5.5 Creation of interlocked media using spheres and flats.** (Harkness 2009)

To model dry stone walls as well and locked sands, Harkness (2009) suggested an alternative means of defining potential functions using only spheres and plane surfaces or ‘flats’. The potential function defining a sphere with \( n \) flats is of the form

\[
f(x, y, z) = (1 - k) \left\{ r_c \left( \sum_{i=1}^{n} \frac{a_i x + b_i y + c_i z + d_i}{\sqrt{a_i^2 + b_i^2 + c_i^2}} \right)^3 \right\} \text{ ellipsoidal term}
\]

\[
+ (1 - k) \sum_{i=1}^{n} \frac{a_i x + b_i y + c_i z + d_i}{\sqrt{a_i^2 + b_i^2 + c_i^2}}^3 \quad \text{n added flats}
\]

\[
+ k r_c^3 \left( \sum_{i=1}^{n} \frac{a_i^2 + b_i^2 + c_i^2}{r_c^2} \right)^{3/2} - 1 \quad \text{added convexity}
\]

(4.7)
\[ r_z = k_r r_z^{desired} \]
\[ r_c = \max(r_x, r_y, r_z) \]

and where \( k_r \) is a user-specified factor (\( 0 < k_r < 1 \)) that relates the desired radii to the scaled radii \((r_x, r_y, \text{and} \ r_z)\) used in the function. Finally, \( s \) and \( k \) are positive constants; \( s \) affects the roundness of the particle corners and \( k \) determines the convexity of any flat surfaces.

This method provides a highly flexible means of constructing arbitrarily shaped particles such as those of railway ballast shown in Figure 4.52 in the previous chapter.

5.2.2. Contact mechanics

In the soft sphere approach, the contact between two particles is generally not a point (Zhu et al. 2007). Instead, it occurs over a finite area and is a function of the degree/state of interpenetration between the contacting pair. However, the resulting stress (or traction) distribution is difficult and computationally expensive to model accurately due to particle geometry, material properties and the transient nature of the particles (Zhu et al. 2007). Subsequently, simplifications are made in calculating the integral of the actual stress acting at the contact. The resulting force at the contact can be decomposed into two components; one normal to the contact plane and one tangential.

The simplest contact constitutive model (or contact model) is what is known as the penalty function (or linear spring) method. The contact force between particle pairs is determined by either relating the area/volume of the overlap to a given particle stiffness or making it equal to the product of the particle stiffness and the magnitude of the overlap (Munjiza 2004). This is however an unrealistic approach when the stiffness changes with the curvature of the particle surface (Harkness 2009), as is the case with potential particles.

A theoretically rigorous alternative commonly used is the Hertz-Mindlin and Deresiewicz model in simplified forms. This is a two part model where the contact mechanics in the normal direction is described by the Hertz (1882) contact model.
of two ellipsoids or spheres, while in the tangential or shear direction it is described by the Mindlin and Deresiewicz (1953) model.

**Normal force**

When using the Hertz model, a number of assumptions are made. These are that the strains induced at the contacts are sufficiently small that the material response remains linear elastic at the contacts; that the contact area between two such elastic ellipsoids is small compared to the particle and of elliptical shape; and that the contacting surfaces are perfectly smooth.

The radius of equivalent spheres in contact can be expressed as

$$R_c = \sqrt{R_a R_b}$$  \hspace{1cm} (4.9)

such that $R_a$ and $R_b$ represent an equivalent ellipsoid in contact

$$R_a = \frac{1}{[(A + B) - (B - A)]} \hspace{1cm} R_b = \frac{1}{[(A + B) + (B - A)]}$$  \hspace{1cm} (4.10)

and

$$A + B = \frac{1}{2(\kappa_{11} + \kappa_{12} + \kappa_{21} + \kappa_{22})}$$  \hspace{1cm} (4.11)
\n$$B - A = \frac{1}{2} \sqrt{(\kappa_{11} - \kappa_{12})^2 + (\kappa_{21} - \kappa_{22})^2 + 2(\kappa_{11} - \kappa_{12})(\kappa_{21} - \kappa_{22})\cos(2\alpha)}$$

$k_{i1}$ and $k_{i2}$ are the major and minor principal curvatures for the $i$th particle. $\alpha$ is the angle between the relative rotation of the axes of major and minor curvature between the two particles.

The secant stiffness at the contact can then be expressed as

$$K_n = \frac{4}{3} E_c \cdot \sqrt{\frac{R_c \delta}{F_2^2}}$$  \hspace{1cm} (4.12)

where $E_c$ is the elastic contact modulus, $\delta$ is the contact overlap and $F_2$ an approximated correction factor that gradually decreases from 1 as the contact becomes more elliptical (Hale 1999) such that,
Finally, the contact normal force at the $i$th timestep can be expressed as

$$F_n^i = K_n^i \cdot \delta$$ \hspace{1cm} (4.14)

**Tangential force**

The shear or tangential component of the contact force is considerably more complicated than the normal component. This is mainly due to the irreversible nature of slips that occur as a result of tangential loading (Johnson 1987). This means that the shear state of a contact at time $t$ is dependent on the loading history (both normal and tangential) associated with that contact.

A number of prominent contact shear models have been formed from the works of Mindlin (1949) and Mindlin and Deresiewicz (1953). These models assume that the tangential force is independent of the normal force, which follows the Hertzian response described previously. Given the non-trivial nature of the Mindlin and Deresiewicz method, researchers have proposed alternatives that are simpler and computationally less expensive to implement.

Cundall’s (1988) elastic/perfectly plastic approach does not take into account the loading, unloading and reloading that may occur in the shear direction as described by Johnson (1987). Instead, the shear force in the elastic region is a function of the cumulative tangential displacement which in turn is dependent on the ‘current’ zero-slip shear stiffness given by

$$K_s = 8G_c F_1 \sqrt[3]{\frac{3R_c R_a F_n}{4E_c R_b}} \frac{1}{\Phi}$$ \hspace{1cm} (4.15)

Since the shear force is measured incrementally, the accumulated shear force from the previous step needs to be rotated by the change in orientation of the contact normal between the previous and current step such that

$$F_{s,rot}^i = \Delta R_{normal} F_{s}^{i-1}$$ \hspace{1cm} (4.16)
where $\Delta R_{\text{normal}}$ is the contact normal rotation matrix between time steps. Then the shear force for the $i$th cycle is

$$F_s^i = F_{s,\text{rot}}^i + K_s^i \cdot \delta_s^i$$  \hspace{1cm} (4.17)

where $\delta_s^i$ is the incremental shear displacement for the $i$th cycle and the limiting conditions are

$$F_s^i := \begin{cases} F_s^i & |F_s^i| \leq |\mu F_n| \\ |\mu F_n| \frac{F_s^i}{|F_s^i|} & |F_s^i| > |\mu F_n| \end{cases}$$  \hspace{1cm} (4.18)

where $\mu$ is the inter-particle friction angle.

### 5.2.3. Simulation cycle for DEM

The simulation cycle in DEM involves repeated application of the law of motion and a force-displacement law implemented through an explicit time integration algorithm.

In the first instance, contacts between particles are updated and the force-displacement law (contact law) is applied to each of the detected contacts. Based on the relative motion between contacting particle pairs, the contact force between them is calculated. The contact force is composed of a normal and shear component. The shear (tangential) component of the contact force will impart a moment and in cases where non-spherical elements are used, so will the normal force component.

The forces and moments are then summed for each particle and the laws of motion used to calculate the rates of change of linear and angular momentum for each particle. These are then integrated together with the translational velocity and rate of change of orientation to obtain the linear and angular momentum and the particle position and orientation for the next cycle. The translational and angular velocities may be calculated from the linear and angular momentum, together with the mass and inertia tensor for each particle. Finally, the time step for the next cycle is calculated and a search for new contacts is performed. The simulation cycle is then repeated. This cycle is illustrated in Figure 5.6.
5. Modelling of Triaxial testing on ballast

Figure 5.6 Typical DEM simulation cycle (O’Sullivan, 2011)
5.3. Specimen preparation

The initial void ratio and packing arrangement contribute greatly to the mechanical response of a DEM specimen. It is therefore important to discuss particle generation and the methods used to attain the desired void ratio and confining pressure.

Preparing a specimen prior to testing is a two-step process. The first step involves the generation of the particles in a large cylinder, followed by the second step of uniaxial compression to the desired boundary stress condition.

In this section, a brief description will be given of how specimens are prepared for the simulation of laboratory triaxial tests on a granular material where the assumed specimen cylinder height of 0.3 m and a diameter of 0.15 m match the dimensions of laboratory specimens.

5.3.1 Distribution of particle size, mass and number

Prior to actual particle generation, adequate consideration must be given to the required Particle Size Distribution (PSD). In laboratory PSD analysis it is assumed that particle size varies linearly between sampling points. This principle is used here to scale the DEM particles to match a given PSD. Parametric information on the desired PSD (sieve sizes and retained mass/percentage) and DEM particles (intermediate dimension and volume) is used in a linear interpolation algorithm to compute scaling factors for each of the particles.

5.3.2 Specimen generation

There are several methods that can be employed to create the initial arrangement of particles; Bagi (2005) and Jiang (2003) provide concise reviews. The Dynamic method of specimen generation is adopted here. A random number generator is used to generate the x, y, and z centroid coordinates for each of the particles within a domain space described by a cylinder measuring 1 m high and 0.15 m in diameter. The cylinder is considered to be rigid (i.e. it has the same stiffness as the particles) and frictionless.
Figure 5.7A: Complex shaped particles are first generated as spheres. B: Particles with the flats turned on.

Using these centroids, particles are generated within the cylinder. The contact stiffness $G$ is set to the desired value that will be used during the testing and inter-particle friction $\phi_\mu$ is set to zero.

The height of the cylinder is exaggerated (i.e. 1 m instead of 0.3 m) so that the available space is large enough to minimise particle overlap which is a common consequence of using random number generators.

Inevitably, there may be a number of particles that overlap each other resulting in undesired contact forces developing between them. While it is possible to discard and regenerate the overlapping particles in a different location, an alternative solution is to run a number of calculation cycles in the presence of damping and allow the overlapping particle to move apart naturally, leaving the randomised particles arrangement intact.

This method can be computationally expensive especially where the specimen has a very large number of complex geometry particles described by potential functions. To account for this, the flat surfaces of the particles are switched off at this stage resulting in the generation of what could be described as circumscribing spherical particles (Figure 5.7A).
The absence of the additional complexity introduced by the flats significantly reduces the time needed to resolve any particle overlap in the system.

The void ratio is then reduced by using a combination of gravitational sedimentation and vertical compression. The sedimentation methodology used is similar to that described in Thomas (1997) and Clayton and Abbireaddy (2009) whereby the loosely dispersed particles are allowed to fall freely under gravity ($g = 9.81 \text{ m/s}^2$). Concurrently, the top (platen) of the cylinder which has been prescribed a mass of 1 kg, is allowed to fall freely for a distance of 0.7m. Figure 5.8 shows a specimen after it has been compressed in this way.

The top platen is used for two reasons. Firstly, it ensures that the top of the specimen is completely flat with the maximum number of particles in contact with the platen. This is required to avoid bedding-in errors during testing. Secondly, it allows the achievement of lower void ratios not otherwise attainable. This process of attaining the desired void ratio for a DEM specimen can be considered analogous to the methods used in the laboratory for preparing specimens consisting of gravel-sized particles, where the granular material is usually poured into a cylindrical mould and vibrated to achieve the desired initial void ratio.

During this process, an inter-particle friction that is smaller than or equal to the final test value can be used to further control the void ratio (Cundall 1988).
If large friction values are modelled during the specimen generation phase, this will result in strong forces developing within the particle matrix as shown in Figure 5.9A. As a consequence, the specimen will effectively be ‘pre-stressed’. This is undesirable as a target confining stress lower than the pre-existing stress state could cause the specimen to explode during testing. A simple but computationally costly solution is to allow the specimen to cycle (with the boundary motion inhibited) until the excess stress is dissipated. Damping can also be introduced to improve computational efficiency.

![Figure 5.9 A: Force chains after initial compression with inter-particle friction B: and after stress relief](image)

Alternatively, the inter-particle friction can be set to zero prior to cycling as a way of relieving stress (Calvetti 2008). This is the method adopted here. It should be noted that a sudden loss of friction will cause a small fraction of particles to rearrange. This is acceptable in the specimen generation stage since the rearrangement of particles will continue during the isotropic compression stage prior to shearing (Ahmed et al. 2014).

Once the required void ratio and height parameters have been reached, the specimen is checked to make sure it is in equilibrium. Finally, the particle configuration information (i.e. particle centroids and geometry) is exported to a file for subsequent use.
5.3.3. Specimen testing

After the initial preparation in a cylinder, the specimen is regenerated with a virtual membrane as shown in Figure 5.13. The frictional and stiffness properties of the top and bottom platen are set.

The specimen is then isotropically compressed to the desired confining pressure. A servo controlled algorithm is used to bring the strain rate monotonically to convergence with the required confining stress (Figure 5.12). This algorithm works by adjusting the strain rate to minimise the error between the current and desired confining pressure. A suitable gain $\alpha_g$ is prescribed so that the rate of loading is slow enough for inertial effects to be negligible. Once the required confining pressure is achieved, the specimen is cycled to equilibrium with all boundary motion inhibited (Figure 5.13). This is sometimes referred to as period of “quiescence” (Kuhn 2006).

While the gravity sedimentation method is able to produce a well packed and fairly homogenous specimen, with increasing inter-particle friction there is a danger of cavities forming within the specimen (Figure 5.10). These ‘loose’ zones will tend, especially in dense specimens, to fail abruptly under strain resulting in what can be described as ‘bedding errors’. It is therefore important to check the homogeneity of the specimen prior to shearing.

The method described by Jiang et al (2003) for the evaluation of homogeneity is adopted here. The specimen is divided into $n$ slices with a thickness of $\geq 2.25$ times the median particle size. The void ratio of $i$th slice is given by $e_i$ and the specimen homogeneity index $S^2$ is defined as,

$$S^2 = \frac{1}{n-1} \sum_{i=1}^{n} (e_i - e)^2$$

(4.18)

where $e$ is the target void ratio. Jiang et al (2003) considered a $S^2$ of $<0.03$ to be adequate to describe a specimen, consisting of spheres/circles, as ‘very homogeneous’. In this case, a lower target homogeneity index $S^2$ of approximately 0.01 is adopted since angular particles will tend to pack closer together resulting
in smaller void space. The specimen is considered ready when the confining pressure, void ratio and total kinetic energy of the system reach steady state. At this point the confining pressure is switched from the servo-controlled algorithm to a fixed pressure and the top and bottom platen are moved towards each other to impose shearing at a given rate.

![Figure 5.10 Formation of cavities within specimen](image)

5.3.4. General remarks on modelling the triaxial cell

A real triaxial cell is not a perfect instrument and must operate within the limitations set by real materials and equipment. One such limitation is the latex membrane, placed around the specimen, which serves as a boundary between the specimen and the confining fluid. Confining pressure is applied via the membrane and changes in the volume enclosed by the membrane are used to determine volumetric strain.

The use of a latex membrane is a practical engineering solution to this problem, but is less than ideal. A particular problem with specimens comprising large particles is that, as the confining pressure is increased, the membrane distorts inwards into the voids between the particles (membrane penetration). This introduces a potentially significant error into the determination of void ratio and volumetric strain. A further undesirable effect is that, as the membrane is stretched and the specimen distorts, it is likely to impose local shear forces on the surface of the specimen together with an additional hoop stress.
Figure 5.11 A: Virtual membrane. B: virtual spheres on platen

Figure 5.12 Confining pressure application

Figure 5.13 stabilisation of total kinetic energy in system
A numerical model is not subject to these physical limitations and a balance needs to be struck between producing an accurate model of a real triaxial cell and a model of an idealized triaxial cell. While it is necessary to produce a model that is reasonably faithful to the real cell, as comparison with the results from real tests is essential for the validation of the numerical model, it would be undesirable to expend excessive effort in simulating the shortcomings of the real system. In general this latter approach to modelling - i.e. an idealised triaxial cell - has been adopted. No attempt was made to model the true behaviour of a latex sheet, concentrating instead on the function of a membrane; the application of confining pressure and the measurement of specimen volume. It is therefore necessary to maintain an awareness of the difference between the real and numerical models when comparing the results.

5.3.5. Analysis parameters

Stresses are effective stresses as defined by Terzaghi. In triaxial compression the major principal effective stress $\sigma'_1$ is the pressure resulting from the force applied in the z direction over the area of the platen. The intermediate principal effective stress $\sigma'_2$ and minor principal effective stress $\sigma'_3$ are equal to the applied confining pressure. The mobilised shear strength $\phi'_\text{mob}$ expresses the maximum ratio of shear stress to normal stress at any plane and is defined as,

$$\phi'_\text{mob} = \sin^{-1} \left( \frac{\sigma'_1 - \sigma'_3}{\sigma'_1 + \sigma'_3} \right)$$

(4.19)

The global axial strain $\varepsilon_a$ is defined as the change of axial height of the specimen divided by the height at the start of the test. The volumetric strain $\varepsilon_{vol}$ is defined as the change of volume of the specimen divided by the initial volume of the specimen. The volume of the specimen is taken to be the volume enclosed by the surface mesh that defines the virtual membrane.

The sign convention adopted here takes compression as positive and dilation as negative in line with soil mechanics convention.

The measurement of void ratio is carried out on an internal cylindrical volume of the specimen as shown in Figure 5.14. The defined internal cylinder is subdivided
into a number of slices taken normal to its axis and the average of these slices is reported.

*Figure 5.14 Internal volume cylinder*
5.4. Parametric study

In this section results are presented from a series of numerical simulations that has been performed to check the capability of the model and the shear behaviour of the potential particle based numerical ballast under triaxial compression.

For a given specimen, there are five principal numerically variable modelling parameters that can influence the results:

1. Time step
2. Shearing speed
3. Damping
4. Contact stiffness
5. Inter-particle friction

Time step and shearing speed are considered as purely numerical parameters whose value needs to be selected to have no significant influence on results. The contact stiffness and inter-particle friction have a physical significance. Their values need to be calibrated to match physical test data for the behaviour of the whole triaxial specimen. Although these parameters could perhaps be measured directly (e.g., Cavarretta et al. 2010), there are significant difficulties in achieving this and no values for ballast are available in the literature. Damping can be considered as both a numerical and physical quantity; however as, in the numerical model, the value is selected so as to have no significant influence on the results, it is not necessary to consider the physical significance of the value used.

The influence of these parameters was studied in turn through a series of simulations detailed in Table 5.1.
Table 5.1 Details of parametric study for numerical tests

<table>
<thead>
<tr>
<th>Simulation Set</th>
<th>Variables</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Numerical</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Mechanical</td>
<td></td>
</tr>
<tr>
<td>Time step</td>
<td>Shearing speed</td>
<td>Damping</td>
</tr>
<tr>
<td>TS1,2 &amp; 3</td>
<td>Varied</td>
<td>0.2m/s</td>
</tr>
<tr>
<td>V4, 5 &amp; 6</td>
<td>0.5</td>
<td>Varied</td>
</tr>
<tr>
<td>D7, 8, 9 &amp; 10</td>
<td>0.5</td>
<td>0.2m/s</td>
</tr>
<tr>
<td>CS11 &amp;12</td>
<td>0.5</td>
<td>0.2m/s</td>
</tr>
<tr>
<td>IF13. 14 &amp;15</td>
<td>0.5</td>
<td>0.2m/s</td>
</tr>
</tbody>
</table>
5.4.1 Effects of time step

The timestep is determined by considering each particle and the system of contacts around it. This sub-system has a mass (i.e. that of the particle) and a stiffness associated with it, so an approximate natural frequency can be calculated for each axis and for the rotational movement. The critical timestep is then related to this natural frequency such that

\[
t_{\text{crit}} = \begin{cases} 
\sqrt{m/k^{\text{tran}}} & \text{(translational motion)} \\
\sqrt{I/k^{\text{rot}}} & \text{(rotational motion)}
\end{cases}
\]  

(4.20)

Where \(k^{\text{tran}}\) and \(k^{\text{rot}}\) are the translational and rotational stiffness, \(I\) is the moment of inertia and \(m\) is the mass (Itasca 2008). This calculation is performed for all the particles in the system and the smallest critical value is taken to be the timestep for the whole system.

The central difference time integration method used here is a conditionally stable algorithm and therefore requires that the size of the time step employed does not exceed a critical timestep \(t_{\text{crit}}\).

Owing to the approximate nature of the mechanically determined critical timestep, a fraction of the calculated critical timestep is used as the actual time increment so that

\[
\Delta t = \alpha_{sf} t_{\text{crit}}
\]

(4.21)

where \(\alpha_{sf}\) is the safety factor. Itasca (2008) recommend \(\alpha_{sf} = 0.80\) for simulations using the linear contact law and 0.25 for simulations using a Hertz-Mindlin contact law.

While the use of a safety factor helps to improve the robustness of the automatic timestep determination, it will increase simulation time and computational cost. For \(\alpha_{sf} = 0.25\), the simulation duration will nominally increase by 400%. It is therefore important to choose an appropriate value for \(\alpha_{sf}\) that balances simulation accuracy and computational cost.
The simulation timestep affects the accuracy of the integration and hence the results obtained from the simulation. It is therefore important to see the effects of timestep size on the outcome of simulations. Three simulations were carried out using safety factors of 0.20, 0.50 and 1.00. The $\alpha_{sf} = 1.00$ is used as the benchmark value.

The specimen was prepared using the method already described (Section 5.2) and only the value of $\alpha_{sf}$ was varied between simulations. (Table 5.2).

The total kinetic energy (i.e. the sum of translational and rotational kinetic energy) of the simulation is commonly used to judge the extent of instabilities that may have been induced during shearing (e.g. Tsuji et al (1993) and Thornton (2000)). Figure 5.15 shows the change in total kinetic energy during shearing while a statistical summary is given in Table 5.3.

An upper limit of $10^3$J for the kinetic energy is used as an indicator of stability since it's sufficiently low enough for the specimen size and particle mass and velocity. The combination of a low mean and standard deviation of the kinetic energy in TS1 suggests that it is comparatively more stable than the other tests. This however comes at a very high computational cost. TS1 needed to run for approximately 64 hours to reach an axial strain of 15%. On the other hand, it took TS2 and TS3 approximately 40 hours and 25 hours, respectively.

Figure 5.16 shows the mobilised strength and volumetric strain behaviour for these tests. The initial response of the three tests is nearly identical. Maximum compression is reached at around 4% axial strain and there is a variation of -1% and 1.4% in TS1 and TS2 respectively when compared with the benchmark (Table 5.2). At an axial strain of 4.7% an event occurs that causes a sharp drop in strength and a concurrent (but smaller) drop in volumetric strain. Since this event affected all three tests at precisely the same axial strain, it can be concluded that this is a feature of the specimen and most likely caused by a slippage resulting in a momentary loss of strength. Inspection of the force chain network just before and after the slip confirms this. The region highlighted by the dashed lines in Figure 5.17 shows how a major force chain is reconfigured as a result of the slip.
Beyond this point, all three tests dilate monotonically with T1 and T2 having similar rates of 0.175 and 0.161 respectively. T3 on the other hand has a lower rate of dilation at 0.120. The peak friction angle, the maximum volumetric strain and the volumetric strain at the end of the test are presented in Table 5.2 and show small variations in response between the three $\alpha_{sf}$ values with T1 and T2 very closely matched. The minor differences seen in these tests are primarily down to the differences in the energy balances of the systems and the similarity between T1 and T2 both in terms of global response and kinetic energy variation (Figure 5.15) seems to confirm this.

Figure 5.18 presents the contact coordination number (CN). T1 has a CN 4.8% and 3.2% greater at an axial strain of 5% and 10%, respectively when compared with the benchmark. On the other hand, the CN for T2 is 1.6% and 0.4% smaller at 5% and 10% axial strain, respectively. These results show that the tested $\alpha_{sf}$ values and by extension the different timesteps have very little effect on the internal configuration of the particles as expressed by the number of contacts being formed.

The data in Figure 5.15 and Table 5.3 show that the timestep affects the results of a DEM simulation. Larger timesteps result in higher kinetic energies, causing vibration of the specimen and leading to a small suppression of dilation due to dynamic rearrangement. The mechanically determined critical timestep may be used as an initial estimate and in this case a safety factor $\alpha_{sf} = 0.5$ provides a balance between stability and computational cost.
5. Modelling of Triaxial testing on ballast

Table 5.2 Differences in strength response for varying timestep. Confining pressure = 200 kPa, inter. friction = 30°, initial void ratio = 0.68 and contact stiffness = 1 GPa

<table>
<thead>
<tr>
<th>Test no.</th>
<th>$\alpha_{sf}$</th>
<th>$\phi'_{peak}$ (°)</th>
<th>Max. $\varepsilon_{vol}$ (%)</th>
<th>Rate of dilation at $\phi'_{peak}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>TS1</td>
<td>0.25</td>
<td>42.18</td>
<td>1.287</td>
<td>-0.554</td>
</tr>
<tr>
<td>TS2</td>
<td>0.50</td>
<td>42.24</td>
<td>1.318</td>
<td>-0.504</td>
</tr>
<tr>
<td>TS3</td>
<td>1.00</td>
<td>41.61</td>
<td>1.300</td>
<td>-0.181</td>
</tr>
</tbody>
</table>

Table 5.3 Energy statistics for different timesteps $\alpha_{sf}$. rates ($\times 10^4$)

<table>
<thead>
<tr>
<th>Test no</th>
<th>$\alpha_{sf}$</th>
<th>Mean TKE (j)</th>
<th>Median TKE (j)</th>
<th>Std. deviation (j)</th>
</tr>
</thead>
<tbody>
<tr>
<td>T1</td>
<td>0.25</td>
<td>0.98</td>
<td>0.83</td>
<td>0.74</td>
</tr>
<tr>
<td>T2</td>
<td>0.50</td>
<td>1.51</td>
<td>1.35</td>
<td>0.861</td>
</tr>
<tr>
<td>T3</td>
<td>1.00</td>
<td>2.01</td>
<td>1.74</td>
<td>1.22</td>
</tr>
</tbody>
</table>

Figure 5.15 Total kinetic energy Vs. axial strain for varying timesteps.
Figure 5.16 Effects of different timesteps on (a) Mobilized friction angle and (b) volumetric strain versus axial strain.
Figure 5.17 Force chain network before (A1) and after slip (A2). Major force chains before (B1) and after slip (B2).

Figure 5.18 Contact coordination number at different timestep safety factors
5.4.2. Effects of shearing speed

The shearing speed of a laboratory triaxial cell experiment on a non-clay soil is typically between 0.5 and 0.001 mm/minute (0.0023 to 0.000006% of the specimen height per second) (Head 1998). To match this rate in the simulation would take too long (i.e. months), owing to the small timestep and the computational work required at each step. Thus faster shear speeds were used in the simulations to reduce the run time to an acceptable level. If the rate of deformation were too fast, the model response would be dynamic representing rapid granular flow rather than the quasi-static behaviour seen in a triaxial test. The chosen shear velocity must therefore be slow enough to induce a quasi-static soil response yet fast enough to give realistic run times.

Triaxial shear tests were carried out using three velocities, i.e. 0.2, 0.02 and 0.002 m/s. It should be noted that both the top and bottom platen move to shear the specimen, resulting in individual platen velocity of half the prescribed relative speed. The test parameters are given in Table 5.1.

The inertia number $I_n$ can be used to assess the nature of the response (plastic/static or visco-plastic/dynamic) and is defined as

$$I_n = \varepsilon_q \sqrt\frac{m}{pd}$$  \hspace{1cm} (4.22)

Where $\varepsilon_q$ is the shearing strain rate, $m$ is the average mass of a particle in the specimen, $p$ is the confining pressure and $d$ is the particle diameter (GDR-Midi 2004; Radjai 2009; O'Sullivan 2011). Previous authors have shown that small inertia numbers correspond to the dense flow regime, associated with a network of enduring contacts in quasi-static regimes (Iordanoff & Khonsari 2004), and larger inertia numbers correspond to the dynamic inertial regimes, seen in rapid flow or binary collision (Roux & Combe 2002). It is recommended that $I_n \ll 1$ for plastic flow.

The maximum inertia numbers for V4, V5 and V6 are $4.19 \times 10^3$, $4.19 \times 10^4$ and $4.19 \times 10^5$, respectively. Assuming a limiting inertia number of $10^2$ (GDR-Midi 2004) this indicates that the response in all three tests is quasi-static. Figure 5.19
shows the effect on the total kinetic energy as a result of varying the rate of shearing. Higher energies are seen in faster tests since the kinetic energy in a system is a function of velocity. Consequently, V4 has the highest average energy and with successive reduction in velocity, a reduction in total kinetic energy in the system is seen. The mean kinetic energy in V4, V5 and V6 is in the order of $10^2$, $10^4$ and $10^5$, respectively. None of the tests showed any signs of abnormal behaviour that would indicated instability in the model.

Figure 5.20 show the mobilised strength and volumetric strain behaviour for the tests. The effect of strain rate on peak friction angle is minimal. Using V5 (0.01 m/s) as a benchmark, it can be seen that peak friction in V4 (0.1 m/s) varies by only 2.77°. While the difference between the benchmark and V6 is minor at 0.66° (Table 5.5). With increasing rate of shear, the maximum compression decreases (not significantly) and the maximum rate of dilation increases. This indicates a transition from loose to dense behaviour as the rate of shear increases.

Figure 5.21 presents the change in contact coordination number with shear rate. It shows that beyond 7% axial strain, the CN for the tests diverge from each other. At an axial strain of 10% the CN for V4 varies by 5.8% compared to the benchmark while V6 has a modest difference of 17.6%.

It is generally acknowledged that DEM simulations on granular models should be run as slowly as possible. It is also understood that if the rate of shear is too slow it can lead to high costs with little gained in terms of fidelity of results. The slowest test presented here took ≈105 hours (4.4 days) to reach an axial strain of 10% but its stress and strain behaviour were not significant difference to other tests. The CN difference between V5 and V6 are negligible. Therefore, a strain rate of 0.02m/s presents the best choice for computational cost and simulation stability.
Table 5.4 Total kinetic energy statistics at different shear rates ($\times 10^3$)

<table>
<thead>
<tr>
<th>Test no</th>
<th>$\varepsilon_q$ (%/s)</th>
<th>Mean TKE (J)</th>
<th>Median TKE (J)</th>
<th>Std. deviation (J)</th>
</tr>
</thead>
<tbody>
<tr>
<td>V4</td>
<td>133</td>
<td>0.14</td>
<td>0.12</td>
<td>2.62</td>
</tr>
<tr>
<td>V5</td>
<td>13.3</td>
<td>4.85</td>
<td>5.23</td>
<td>1.23</td>
</tr>
<tr>
<td>V6</td>
<td>1.33</td>
<td>4.89</td>
<td>4.91</td>
<td>1.49</td>
</tr>
</tbody>
</table>

Table 5.5 Variation in response induced by different strain rates. Confining pressure = 15 kPa, inter. friction = 40°, initial void ratio = 0.61 and contact stiffness = 1 GPa

<table>
<thead>
<tr>
<th>Test no</th>
<th>$\varepsilon_q$ (%/s)</th>
<th>$\phi'_\text{peak}$ (°)</th>
<th>Max. $\varepsilon_{vol}$ (%)</th>
<th>Rate of dilation at $\phi'_\text{peak}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>V4</td>
<td>133</td>
<td>52.44</td>
<td>0.136</td>
<td>0.833</td>
</tr>
<tr>
<td>V5</td>
<td>13.3</td>
<td>49.67</td>
<td>0.145</td>
<td>0.717</td>
</tr>
<tr>
<td>V6</td>
<td>1.33</td>
<td>49.01</td>
<td>0.153</td>
<td>0.655</td>
</tr>
</tbody>
</table>

Figure 5.19 Effects on total kinetic energy due to varying shear rates.
Figure 5.20 Effects of different shear rates on (a) Mobilized friction angle and (b) volumetric strain versus axial strain.
Figure 5.21 Contact coordination number for varying strain rates
5.4.3. Effects of Damping

When a granular material is strained, kinetic energy is dissipated at the contacts through a combination of microscopic processes such as friction and yielding of surface asperities. The contact models used in DEM are highly idealised and therefore incapable of capturing the complex processes that occur in natural materials. Also their elastic nature tends to induce unnatural vibrations. Consequently, damping is commonly used to control any non-physical vibration that may arise due to excess kinetic energy in a DEM model.

The damping formulation used here is based on the local damping proposed by Cundall (1987) in which the damping force at each particle contact is proportional to the magnitude of the out-of-balance-force with a sign that ensures that the vibrational modes are damped. The damping force is given by,

\[ F_d^i = -\alpha_d |F_0^i| \text{sign}(V^i) \]  

(4.23)

where \( \alpha_d \) is the damping constant, \( |F_0^i| \) is the magnitude of the out-of-balance force for the \( i \)th degree of freedom \((i = 0,1,2)\), \( V^i \) is the velocity of the particle and \( \text{sign}(\cdot) \) indicates the sign (positive or negative) of the particle velocity (Itasca 2008; Potyondy & Cundall 2004).

Three values of damping coefficient \((\alpha_d = 0.05, 0.1 \) and \(0.7)\) were investigated in addition to a simulation in which damping was switched off \((\text{i.e. } \alpha_d = 0)\), as summarized in Table 5.6. An equivalent value of the fraction of critical damping ratio, \( \zeta \), is also given, based on the approximation \( \zeta \equiv \alpha_d / \pi \), valid for low values of damping (Itasca, 2008). The same initial specimen was used for all four tests. After the desired confining (cell) pressure had been applied, the damping constant was changed and the model was cycled to equilibrium, bringing the specimen into a steady state under the new damping conditions.

Figure 5.22 shows the mobilized strength and volumetric strain as a function of shear strain for simulations D7-D10. Damping affects both the strength and the volume characteristics of a specimen. Increasing the damping results in an increase
in peak mobilised friction angle and rate of dilation (Table 5.6). Similar findings were also reported by Ng (2006).

The contact coordination numbers for the tests are presented in Figure 5.23. It can be seen that the number of contacts tends to be higher at the same strains with increased damping. This is related to the rate of dilation and is reminiscent of behaviour seen in the shearing rate tests.

The effect of damping on the total kinetic energy can be seen in Figure 5.24. The difference in average kinetic energy in the system can be found in Table 5.7. As expected higher damping results in lower energy. The difference for D8, D9 and D10 are 4.8%, 7.9% and 18.1%, respectively when compared to the benchmark. Overall, the results strongly suggest that the principal form of energy dissipation is in overcoming contacts and frictional sliding rather than loss through artificial damping.

It is evident that any amount of damping will affect the observed response in DEM simulations of triaxial cells test. It is a parameter that is difficult to relate to a physical phenomenon or property. This should be kept in mind when selecting an appropriate damping factor.

A damping constant of 0.7 is clearly too high and has a dramatic impact on the model response. On the other hand, zero damping is inadvisable when idealized elastic/perfectly plastic contact models are used that have a tendency to induce vibration prior to contact sliding. A range of $\alpha_d$ of between 0.05 and 0.1 is suitable in this case, as it ensures specimen stability but has only a small influence on the soil response.

<table>
<thead>
<tr>
<th>Test no.</th>
<th>$\alpha_d$</th>
<th>approximate equivalent damping ratio, $\zeta \cong \frac{\alpha_d}{\pi}$</th>
<th>$\phi_{peak}$ ($^\circ$)</th>
<th>Max. $\epsilon_{vol}$ (%)</th>
<th>Rate of dilation at $\phi_{peak}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>D7</td>
<td>0.00</td>
<td>0.000</td>
<td>47.72</td>
<td>0.143</td>
<td>0.578</td>
</tr>
<tr>
<td>D8</td>
<td>0.05</td>
<td>0.016</td>
<td>47.86</td>
<td>0.145</td>
<td>0.595</td>
</tr>
<tr>
<td>D9</td>
<td>0.10</td>
<td>0.031</td>
<td>49.54</td>
<td>0.195</td>
<td>0.826</td>
</tr>
<tr>
<td>D10</td>
<td>0.70</td>
<td>0.223</td>
<td>54.21</td>
<td>0.189</td>
<td>0.714</td>
</tr>
</tbody>
</table>

*Table 5.6 Variation in response caused by different damping constants. Confining pressure=15kPa, inter-particle friction=35$^\circ$, initial void ratio = 0.61 and contact stiffness = 1 GPa*
Table 5.7 Energy balance statics ($10^3$)

<table>
<thead>
<tr>
<th>Test no.</th>
<th>Mean TKE (j)</th>
<th>Median TKE (j)</th>
<th>Std. deviation (j)</th>
</tr>
</thead>
<tbody>
<tr>
<td>D7</td>
<td>4.10</td>
<td>4.17</td>
<td>0.837</td>
</tr>
<tr>
<td>D8</td>
<td>3.90</td>
<td>3.96</td>
<td>0.774</td>
</tr>
<tr>
<td>D9</td>
<td>3.76</td>
<td>3.75</td>
<td>0.764</td>
</tr>
<tr>
<td>D10</td>
<td>3.35</td>
<td>3.43</td>
<td>0.520</td>
</tr>
</tbody>
</table>
Figure 5.22 Effects of damping on (a) mobilized shear strength. (b) the volumetric strain versus axial strain.
Figure 5.23 CN variation at different damping constants.

Figure 5.24 total kinetic energy at different damping constants.
5.44. Effects of contact stiffness

For Hertzian contacts, the inter-particle stiffness $K$ is a function of the particle material shear modulus, $G$, and the effective radius of curvature local to the contact. For rough surfaces, this radius of curvature may be much smaller than the idealized, smooth, particle shapes and there is therefore some uncertainty in the choice of the stiffness value. To assess the influence of shear modulus on the response of the model, simulations were carried out with $G=1$ GPa and $G=10$ GPa.

The contact stiffness at which a specimen is brought to equilibrium can affect the configuration of the particle matrix i.e. its fabric. To avoid any drastic variation in the fabric between the two specimens, the contact stiffness of test CS11 (see Table 5.1) was changed and cycled to equilibrium with all boundary motion inhibited (e.g. Calvetti (2008) and Ng (2006)). A small change in the void ratio was registered (Table 5.8) along with minor movements in the particle matrix. The average displacement of particles was at $6.1 \times 10^{-4}$ unit lengths, representing a movement of $0.0002\%$ of the average particle diameter. Although small, this may cause some contacting particles to be pushed apart, affecting the initial contact coordination number.

It can be seen from Figure 5.25 that changes in the stiffness of the contacts have an effect on mobilised strength. While the peak strengths are similar (with a difference of less than $1\%$), the initial response is distinctly different. This can be explained by the differences in volumetric strain behaviour between the two tests. Increasing the contact stiffness reduces the potential for a specimen to compress, inhibiting rearrangement of the particles to a denser state. Consequently, stiffer behaviour is seen in the initial response of mobilized effective friction angle against shear strain.

The contact coordination number is also affected. Figure 5.26 shows a reduction of $CN$ with an increase in contact stiffness. This is not unexpected as higher stiffness will inhibit closer packing due to the reduced interpenetration, thus reducing the number of contacts forming in the specimen. Furthermore, the rate of change of CN will also be affected; with higher $G$ the particle matrix will be
stronger and less susceptible to rearrangement. Similar overall findings have been reported by various authors (e.g. Cho et al (2007), Potyondy & Cundall (2004), Ng (2006) and Calvetti et al. (2003)).

The critical timestep is related to the contacts stiffness through Equation 4.20 and in general any increase in stiffness will adversely affect simulation duration. The higher stiffness value was found to double total simulation time. Therefore, the lowest practical value for $G$ would be recommended.

<table>
<thead>
<tr>
<th>Test no.</th>
<th>Void ratio</th>
<th>Contact stiffness (GPa)</th>
<th>$\phi_{\text{peak}}$ (°)</th>
<th>Max. $\epsilon_{\text{vol}}$ (%)</th>
<th>Rate of dilation at $\phi_{\text{peak}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CS11</td>
<td>0.67</td>
<td>1</td>
<td>41.61</td>
<td>1.30</td>
<td>0.132</td>
</tr>
<tr>
<td>CS12</td>
<td>0.68</td>
<td>10</td>
<td>42.21</td>
<td>0.71</td>
<td>0.667</td>
</tr>
</tbody>
</table>

*Table 5.8 Variation in response caused by different contact stiffnesses. Confining pressure=200 kPa and inter-particle friction angle=30°*
Figure 5.25 Effect of contact stiffness variation on (a) Mobilized shear strength and (b) Volumetric strain versus axial strain
5.4.5. Effects of inter-particle friction

Three values of inter-particle friction angle $\phi_\mu$ were tested to assess its effect on the mechanical response of the model. The testing parameter values used are given in Table 5.1. The settled specimen for IF15 was used as the initial specimen for the other tests. The inter-particle friction angle was reduced to the required level and the model was allowed a period of quiescence in order to bring it to equilibrium.

While there was no change in the initial void ratio, specimens prepared in this way will be prone to changes in contact state and force chain configuration during shear. Contacts that were initially stable (at the higher $\phi_\mu$) will inevitably become closer to sliding as $\phi_\mu$ is decreased. However, even by the end of the shear test simulation with the largest change (i.e. IF15), only 0.003% of contacts had changed state.
Figure 5.27 shows the behaviour expected of a granular material as the inter-particle friction angle is increased, with generally higher peak strengths being mobilised at a lower axial strain. The initial rate of compression is reduced, dilation starts at a smaller strain and the rate of dilation is increased. The number of sliding contacts reduces with increasing inter-particle friction angle, with IF15 ($\phi_\mu = 40^\circ$) having 63% fewer at 16% axial strain, and IF 14 ($\phi_\mu = 35^\circ$) having 38% fewer than IF13 ($\phi_\mu = 30^\circ$) (Table 5.10 and Figure 5.28). Reducing $\phi_\mu$ promotes an apparently less stiff and less dilatant response and could be used as a proxy for particle abrasion and breakage, which is argued by McDowell and de Bono (2013) to be responsible for the reduction in peak strength, stiffness and dilation of soils with increasing confining (cell) pressure.

<table>
<thead>
<tr>
<th>Test no.</th>
<th>$\phi_\mu$ (°)</th>
<th>$\phi_{peak}$ (°)</th>
<th>Max. $\epsilon_{vol}$ (%)</th>
<th>Rate of dilation at $\phi_{peak}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>IF13</td>
<td>30</td>
<td>46.69</td>
<td>0.30</td>
<td>0.387</td>
</tr>
<tr>
<td>IF14</td>
<td>35</td>
<td>48.03</td>
<td>0.17</td>
<td>0.554</td>
</tr>
<tr>
<td>IF15</td>
<td>40</td>
<td>49.77</td>
<td>0.14</td>
<td>0.730</td>
</tr>
</tbody>
</table>

Table 5.9 Variation in response induced by different inter particle friction. Confining pressure = 15 kPa, initial void ratio = 0.61 and contact stiffness = 1 GPa

Table 5.10 Changes in contact mechanics induced by different inter particle friction. Measurements were taken from an internal cylinder.

<table>
<thead>
<tr>
<th>Test no.</th>
<th>No. contacts in ROI</th>
<th>Average force (N)</th>
<th>Number. sliding</th>
</tr>
</thead>
<tbody>
<tr>
<td>IF13</td>
<td>6164</td>
<td>8.127</td>
<td>1428</td>
</tr>
<tr>
<td>IF14</td>
<td>5543</td>
<td>8.855</td>
<td>889</td>
</tr>
<tr>
<td>IF15</td>
<td>5035</td>
<td>9.034</td>
<td>535</td>
</tr>
</tbody>
</table>

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Figure 5.27 The effects of variation in inter-particle friction on (a) Mobilized shear strength and (b) Volumetric strain versus axial strain
Figure 5.28 The effects of variation in inter-particle friction on average contact coordination number
5.5. Model calibration

It is generally accepted that DEM models are able to replicate the fundamental responses (e.g. dilatancy, shear localisation, stress dependence, etc.) of granular media. The input parameters that dictate this response can be broadly classified into geometrical properties (particle shape and size distribution) and mechanical properties (type of contact model, contact stiffness and friction).

Recent advances in modelling particle geometry have meant that researchers are no longer restricted to using simple sphere or clumps of spheres. As shown in Chapter 4, concepts such as potential particles (Harkness 2009) can be used to create DEM particles that are quantifiably analogous to real materials. Similarly, the implementation of realistic PSD’s in simulations is common place.

This, however, is not the case when considering the mechanical properties. Whilst it is tempting to use real values for contact stiffness and inter-particle friction, they are notoriously difficult to measure accurately and there is little available data on real materials. Furthermore, the simplification of the complex contact mechanics inherent in real granular systems means that there is no guarantee of accurately capturing the response using measured values.

As a result, the accepted approach is to calibrate the mechanical inputs for a numerical material with reference to a laboratory experiment, such that the simulation is able to capture the observed macro-scale response.

5.5.1. Calibration method

The calibration process consisted of matching, as closely as practically possible, the macroscopic behaviour of the DEM model to that of laboratory triaxial cell experiments performed under similar boundary conditions. The parameters calibrated included the inter-particle contact stiffness $K$ and inter-particle friction angle $\phi_{\mu}$. The method used here is similar to that described by Belheine et al. (2008).

A simple two-step procedure was used. First, adjustments were made to the inter-particle friction angle until the volumetric strain behaviour of the real material was captured. At the same time the peak friction angle $\phi'_{\text{peak}}$ was also monitored
as a means of measuring the suitability of the adjustment. Lastly, the contact
stiffness was varied to reflect the deformation characteristics seen in the
laboratory results.

The benchmark laboratory triaxial cell experiments was carried out on 1/3 scaled
ballast (i.e. BS EN 13450:2002 grading category A scaled by 1/3) sourced from
Cliffe Hill quarry (Aingaran, 2014). The specimen dimensions were 300 mm high
and 150 mm diameter. It was sheared monotonically under a confining pressure
of 15 kPa at a rate of $8.33 \times 10^6$ m/s. CT image analysis showed that unloaded
laboratory specimens had a void ratio of 0.65 and approximately 2800 particles.
The DEM model was prepared as previously described, matching the dimensions,
PSD, number of particles and the void ratio as closely as possible.

5.5.2. Calibrated model parameters.
The parameter values obtained by calibration are summarized in Table 5.11. The
results of triaxial test simulations carried out using these parameters are
compared with laboratory test data from two tests at 15 kPa confining pressure
in Figure 5.29. Agreement is very close, with the calibrated model capturing both
the strength and dilatancy characteristics of the real material. There is a small
variation in the laboratory data and the simulation lies, on the whole, in the same
range. Comparative ratios (experimental/DEM) of peak strength $\phi'_\text{peak}$, critical
state strength $\phi'_\text{crit}$ and rate of dilation are given in Table 5.12. They indicate
that the numerical model is able to match the peak and critical state behaviour
with an error of 2%.

Figure 5.30 compare a DEM simulation carried out at 30kPa using the calibrated
parameters to a laboratory experiment at the same confining pressure (Aingaran,
2014). Although the overall behaviour is very similar, the DEM specimen
undergoes additional compression followed by a higher rate of dilation (Table
5.12). This translated into slightly higher peak and critical state strength.
Nonetheless, the DEM simulation can be considered a good fit with the laboratory
result.
### Table 5.11 Calibration model parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inter-particle friction angle $\phi_\mu$</td>
<td>$40^\circ$</td>
</tr>
<tr>
<td>Contact stiffness $K$</td>
<td>1GPa</td>
</tr>
<tr>
<td>Particle Density $\rho$</td>
<td>2650kg/m$^3$</td>
</tr>
<tr>
<td>No. of particles</td>
<td>2780</td>
</tr>
<tr>
<td>Void ratio $e$</td>
<td>0.61</td>
</tr>
<tr>
<td>Shear velocity</td>
<td>0.02m/s</td>
</tr>
<tr>
<td>Damping constant $\alpha_d$</td>
<td>0.05</td>
</tr>
<tr>
<td>Timestep safety factor $\alpha_{sf}$</td>
<td>0.5</td>
</tr>
<tr>
<td>Specimen dimensions</td>
<td>294mm×150mm</td>
</tr>
</tbody>
</table>

### Table 5.12 Comparative ratios (experimental/DEM) between the calibrated DEM model and laboratory element test results

<table>
<thead>
<tr>
<th>Test</th>
<th>$\phi'_\text{peak}$</th>
<th>$\phi'_\text{crit}$</th>
<th>Rate of dilation</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEM</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Lab_15-1</td>
<td>0.98162</td>
<td>1.02253</td>
<td>1.08762</td>
</tr>
<tr>
<td>Lab_15-2</td>
<td>1.00024</td>
<td>1.02384</td>
<td>1.01268</td>
</tr>
<tr>
<td>Lab_30</td>
<td>0.91520</td>
<td>0.95387</td>
<td>0.81056</td>
</tr>
</tbody>
</table>
Figure 5.29 Comparison of DEM and two laboratory experiments (at 15kPa) results
Figure 5.30 Comparison of DEM and laboratory experiments results at 30kPa
5.6. Summary

A new method has been proposed for simulating the behaviour of railway ballast in monotonic triaxial tests, using the innovative 3D potential particle approach and the well-known discrete element method. The elemental particles, PSD and number of particles in each numerical specimen all matched closely the ballast material being modelled.

A parametric study was carried out to investigate the effect on the results of the simulation of five parameters: timestep, shearing velocity, damping, contact stiffness and inter-particle friction. The first three of these are associated with the numerical modelling approach, and the criterion for selecting a particular value is that the value chosen should neither influence the results of the simulation unduly nor make the simulation inefficient or overly expensive in terms of time or computational power.

It was found that the automatically determined timestep is best multiplied by a safety factor of 0.5. This provided the best combination of performance and negligible effect on the results.

The shearing rate presents a special problem when simulating triaxial cell tests of granular materials using DEM as realistic strain rates are impossible to simulate in practicable times. Shearing velocities as low as $10^4$ units has been reported in the literature but this has been at the expense of realistic particle geometry and numbers (e.g. Ng (2006)). It was found that a velocity less than 0.02m/s (or 6.66% strain/s) did not affect the overall response adversely.

Results showed that damping should ideally be kept as low as possible since it not only affects the response of the material but also adversely influences the duration of the simulation. A range of 0.05 to 0.1 was shown to have minimal effect in both these respects.

Contact stiffness was shown to affect both the void ratio and the coordination number, even for specimens whose initial conditions were nearly identical. It is suggested that an increase in particle stiffness will be balanced by a lower coordination number such that the elastic modulus of the particle matrix remains
near constant. Further, its influence on the simulation duration will have a bearing on the value chosen.

The simulations have shown that increasing the inter-particle friction angle will increase the peak strength, and decrease the CN and the percentage of sliding contacts. This demonstrates that friction acts, primarily, to restrict motion and in turn restrict compression through particle rearrangement. With increased friction, individual contacts are less likely to slip (under the same macroscopic strain) increasing the stability of the system and reducing the number of contacts needed to withstand shearing.

Following calibration for the inter-particle friction angle and contact stiffness parameters, the model was able to reproduce satisfactorily the overall response of a scaled ballast in a monotonic triaxial shear test. Very close agreement was achieved in the mobilized strength/shear strain, volumetric strain/shear strain and mobilized strength/rate of dilation behaviour.
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6

Modelling the effects of particle shape

6.1. Introduction
In the past three decades there has been intense research into many fundamental aspects of granular media using DEM with spheres (disks in 2D) as a simplified particle shape. The popularity of the approach stems from the relative ease in identifying whether the spheres (or disks) are contacting. If they are, the geometry of the contact point, including the contact overlap (or separation), can be accurately calculated. Since contact detection is usually the most resource intensive part of a DEM algorithm, the efficiency gained in using spheres can be exploited to achieve realistic particle numbers. However, the excessive freedom of the spherical particles to rotate compared with real soils affects both the dilation that takes place during deformation and the shear strength of soil (e.g. Thornton 2000; Mitchell & Soga 2005; Rothenburg & Bathurst 1992; Iwashita & Oda 1998; Bardet & Proubet 1991). Many authors (e.g. Ng & Dobry 1992; Iwashita & Oda 1998; Ni et al. 2000) have tried to overcome this problem by inhibiting the rotational freedom of spherical particles. This however involves a rather artificial parameter that cannot be related easily or directly to the physical properties of real soil particles.

Spheres remain popular in 3D DEM applications (O’Sullivan 2011). However, the increasing affordability of computational resources has spurred research into modelling complex particle geometry under four broad headings – ellipsoids,
sphere clumps/agglomerates, polyhedra and potential particles (implemented here to create the DEM ballast particles).

Ting et al. (1993) used elliptical particles and Lin & Ng (1997) used 420 ellipsoids to demonstrate that particle shape had a significant effect on specimen strength and internal fabric. Elliptical/ellipsoidal particles have the advantage that the branch and contact vectors between two contacting particles are not collinear. As a result particles are able to transfer moment through the contact normal of the contact force (unlike spheres). Consequently, artificial restriction of rotation is no longer necessary. However, in contrast to the irregular shape of real granular material, particle shapes are still highly idealised.

Thomas & Bray (1999) used 468 clusters of bonded discs to investigate shear resistance and particle rotation in 2D simulations of biaxial tests. Powrie et al. (2005) extend this concept to 3D using spheres and then went on to investigate the effects of particle shape factor on void ratio and strength of granular media in plane strain. Lim and McDowell (2005) used 8-ball clumps/agglomerates to investigate the effects of particle breakage in railway ballast. They found that non spherical particles behaved more realistically due to the interlocking. The concept of clumping spheres together to create complex shapes is growing in popularity since contact detection remains simple and improvements in optimisation continue. For example, Ferrellec and McDowell (2008; 2010) used clumps consisting of as many as 5500 spheres to generate highly realistic particle shapes (Figure 6.1). The main drawback of this method lies in the inverse relationship between accuracy in reproducing particle shape and number of particles. As the individual particles (or clump) become more realistic, the total number of particles in a specimen has to reduce to maintain realistic simulation times. With reducing specimen size, artefacts such as boundary layer effects will have increasingly significant impact on the results (Maynar & Rodriguez 2005; Kuhn & Bagi 2009). Periodic boundaries can be used to mitigate the effects of the boundary although other issues such as correlations between opposite sides of the cell can develop (Pöschel & Schwager 2005).
The use of polyhedral particles is also found in the literature. For example, Azéma et al. (2009) compared the packing characteristics of spheres and polyhedra. They concluded that the faceted nature of the polyhedral particles is responsible for their aggregate strength characteristics. The algorithms associated with polyhedra are more complex with more calculations involved, making them expensive computationally (Pöschel & Schwager 2005; Ferellec & McDowell 2010).

While there is an ever growing body of literature associated with particle shape and DEM, no concerted effort has been made to understand the implications of particle shape characteristics such as form and angularity and their interrelation.

In this chapter, models composed of spheres and ellipsoids will be compared to examine the influence of particle form on the mechanical response of ballast. The influence of angularity will be investigated by comparing specimens composed of ellipsoidal particles and DEM ballast particles. Finally, the idea of particle concavity (i.e. the degree to the sides of a ballast particle curve inward) is introduced and its mechanical influence is explored.

![Figure 6.1 Real ballast particle (left) and models with decreasing number of spheres from left to right. (Ferellec & McDowell 2010)](image)
6.2. A comparison between superquadric and realistic shapes

DEM simulations were carried out on specimens made from spherical and ellipsoidal particles. A third simulation was performed on specimens created from the DEM ballast developed in Chapter 3.

All specimens were prepared as described in Section 4.2, using the calibrated model parameters given in Table 6.1. The target confining stress was set to 200kPa. Vertical slices through the specimens are shown in Figure 6.2. All specimens have a PSD similar to BS EN 13450:2002 grading category A, scaled to 1/3 of full size.

In typical DEM models composed of spherical particles with ordinary contacts (i.e. without rotational springs), it is necessary to restrict particle rotation in order to reproduce quantitatively the behaviour of real granular soils (e.g., Ni et al. 2000; Calvetti 2008). This was not implemented here and particles in the spherical particle specimen (SPS) were free to rotate about all three axes.

For the ellipsoidal particle specimen (EPS) the particle diameters are set to the longest, intermediate and shortest diameters measured from the Cliffe Hill ballast in Chapter 4. This means that the ellipsoid specimen particles have the same form characteristics as the real ballast i.e. the flatness, elongation and equancy ratios are the same.

The bulk densities and void ratios of the specimens are given in Table 6.2. The void ratio was measured using the same method as the resin impregnated laboratory triaxial test specimens (in Section. 3.4) whereby an internal cylindrical volume is sampled. The initial void ratio of all three specimens closely matches the void ratio measured from the unloaded laboratory test specimen in Chapter 3 i.e. $e = 0.61$. 
Table 6.1 Calibrated modelling parameters used in all tests

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inter-particle friction angle $\phi$</td>
<td>40°</td>
</tr>
<tr>
<td>Contact stiffness $K$</td>
<td>1GPa</td>
</tr>
<tr>
<td>Particle Density $\rho$</td>
<td>2650kg/m$^3$</td>
</tr>
<tr>
<td>Shear velocity</td>
<td>0.02m/s</td>
</tr>
<tr>
<td>Damping constant $\alpha_d$</td>
<td>0.05</td>
</tr>
<tr>
<td>Timestep safety factor $\alpha_{sf}$</td>
<td>0.5</td>
</tr>
<tr>
<td>Specimen dimensions</td>
<td>294 mm×150 mm</td>
</tr>
</tbody>
</table>

Table 6.2 Initial void ratio and bulk density for each of the specimens.

<table>
<thead>
<tr>
<th>Specimen Type</th>
<th>Void ratio</th>
<th>Bulk density $\rho_b$ (kg/m$^3$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spheres</td>
<td>0.62</td>
<td>1.6496×10$^3$</td>
</tr>
<tr>
<td>Ellipsoids</td>
<td>0.63</td>
<td>1.5918×10$^3$</td>
</tr>
<tr>
<td>DEM ballast</td>
<td>0.61</td>
<td>1.7078×10$^3$</td>
</tr>
</tbody>
</table>

Table 6.3 Differences in strength response due to form and angularity. Confining pressure = 200 kPa, inter. friction = 40° and contact stiffness = 1 GPa

<table>
<thead>
<tr>
<th>Specimen Type</th>
<th>Ini. void ratio</th>
<th>Peak friction angle (°)</th>
<th>Max. volumetric strain (%)</th>
<th>Rate of dilation at $\phi'_{peak}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spheres (SPS)</td>
<td>0.62</td>
<td>31.2</td>
<td>0.282</td>
<td>0.362</td>
</tr>
<tr>
<td>Ellipsoids (EPS)</td>
<td>0.63</td>
<td>41.8</td>
<td>0.805</td>
<td>0.404</td>
</tr>
<tr>
<td>DEM ballast(DBS)</td>
<td>0.61</td>
<td>52.6</td>
<td>0.826</td>
<td>0.802</td>
</tr>
</tbody>
</table>

Figure 6.2 Internal slice taken from specimen made up of: (A) spherical particles (B) ellipsoidal particles and (C) potential particles
6.2.1 Results

**Stress - strain behaviour**

Figure 6.3 shows the effects of particle shape (form and angularity) on the rate of mobilisation of the angle of friction \( \Phi'_\text{mob} \) and the volumetric strain \( \varepsilon_{\text{vol}} \) with axial strain \( \varepsilon_a \).

As expected, spheres do not reproduce well the behaviour of complex-shaped granular media such as ballast. Their unitary form (i.e. \( S/I = I/L = S/L = 1 \)) and lack of angularity means they are unable to form strong interlocked structures needed to resist shearing. Densification occurs by a small amount until the rolling resistance of the system is overcome. This is followed by dilation where rolling (not sliding, since rotation is not inhibited) is the primary mode of particle rearrangement (discussed later in Figure 6.9). A critical state is reached very quickly as a result. The \( \Phi'_\text{peak} \) of \( 31^\circ \) achieved in this test agrees well with evidence in the literature which suggest that spherical assemblies, where rotation is not artificially impeded, are characterized by very low peak friction angles (\( \approx 30^\circ \)) irrespective of the inter-particle friction angle (Ni et al. 2000; Suiker & Fleck 2004; Calvetti et al. 2004; Calvetti 2008).

EPS exhibits higher strength characteristics compared to the sphere only specimen. For example, the peak strength is over a third greater than that of spheres (Table 6.3). The ellipsoid specimen also compresses nearly three times as much as the SPS (Table 6.3). The rate of dilation at peak strength on the other hand is only slightly higher (\( \approx 10\% \)) indicating that particle form primarily changes the compressive behaviour of granular media which in turn is expressed as a greater resistance to shearing. This is a reasonable conclusion since Donev et al. (2004) have shown that shapes that have non-unitary form (i.e. \( S/I \neq I/L \neq S/L \neq 1 \)) are able to reach a higher density than spheres in random or disordered packing.
Figure 6.3 (A) The mobilised shear strength and (B) volumetric strain against axial strain. $\sigma_3 = 200\text{kPa}$, $\phi_\mu = 40^\circ$, $K = 1\text{GPa}$
Table 6.4 The axial strain $\varepsilon_a$ at maximum strength and maximum compression

<table>
<thead>
<tr>
<th></th>
<th>$\varepsilon_a$ at $\phi'_\text{peak}$ (%)</th>
<th>$\varepsilon_a$ at max. $\varepsilon_{\text{vol}}$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sphere</td>
<td>9.0293</td>
<td>1.3538</td>
</tr>
<tr>
<td>Ellipsoid</td>
<td>9.9278</td>
<td>2.3959</td>
</tr>
<tr>
<td>DEM ballast</td>
<td>6.1201</td>
<td>2.1634</td>
</tr>
</tbody>
</table>

The DEM ballast specimen (DBS) shows the greatest resistance to shearing of the three shapes. Based on the peak mobilised effective friction angle, it can be seen that specimens composed of particles incorporating both form and angularity are 26% stronger than those of particles with form only (i.e. EPS) and 68.8% stronger than a specimen made up of spherical particles. The volumetric behaviour observed with DBS is very similar to that of ellipsoids where specimen densification peaks at 0.826% just after 2% axial strain. Volume expansion takes place thereafter at a rate of dilation that is more than double in comparison with the two other particle shapes (Table 6.3).

Overall, the results show that macroscopic shear strength increase as the constituent particles of a specimen deviate from a regular shape. Several authors have provided experimental evidence to this effect (e.g., Koerner 1970; Guo & Su 2007). Particle form appears primarily to affect the compressive or packing characteristics, while particle angularity has a much greater influence of the dilatant behaviour of a granular mass.

Contact mechanics

Figure 6.4 shows the change in the contact coordination number ($CN$) associated with the different shape of particles in each test. At an axial strain of 0% and the same void ratio in each specimen, the $CN$ is 4.85, 5.56 and 6.24 for SPS, EPS and DBS respectively. The contact coordination number measured from laboratory (triaxial apparatus) specimens, using X-ray tomography, was 6.78 at 0% axial strain at a void ratio of 0.61 (Table 3.6). As the specimens were sheared, the $CN$ started to reduce at a rate apparently connected with the dilatancy of the specimen. Beyond 15% axial strain, all three simulations underwent constant volume shearing and the $CN$ remained essentially constant between 4.5 and 5. Thornton (2000) suggests that this critical $CN$ is a result of the percolation
threshold\(^1\) of the granular mass that satisfies the underlying physical stability of the granular mass.

The fact that a DEM simulation can provide information on the particle interactions and contact forces is central to its use in advancing the understanding of particulate material response (O’Sullivan 2011; Kuhn 1999). The convention generally adopted to visualize the contact forces is to draw a line between the centroids of contacting particles, the thickness of which is proportional to the magnitude of the force. The resulting image is one of a highly complex web or network, which is referred to here as the contact force network.

![Graph](image)

**Figure 6.4 Evolution of contacts coordination number CN with axial strain**

---

\(^1\) This relates to percolation theory which describes the formation of long-range connectivity in random systems. Below the threshold a giant connected component does not exist; while above it, there exists a giant component of the order of the system size

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Figure 6.5 illustrates the evolution of the contact force network for the three specimens with the different particle shapes at three values of axial strain ($\varepsilon_a = 0\%$, $\varepsilon_a = 5\%$ and $\varepsilon_a = 15\%$). The force chain density appears to reduce with increasing realism of shape. This is most evident in the contact force networks at $\varepsilon_a = 0\%$ i.e. prior to loading. This is likely a consequence of the different average number of contacts that are present in the different specimens and therefore the average contact force.

Figure 6.6 plots the distribution of all the contacts and their associated force magnitude in the tested specimens at $\varepsilon_a = 5\%$ and $\varepsilon_a = 15\%$. The radius of the circle, representing the centroid of the contact point, is proportional to the magnitude of the force. The quivers/arrows visualise the top 15\% (or 85\textsuperscript{th} percentile) of the contact force vectors. As the specimens are sheared (5\% axial strain), the development of anisotropy becomes more pronounced with increasing shape complexity i.e. fewer force chains take up the majority of the load. The contact forces in SPS are better distributed with a distinct lack of a strong (or dominant) force chain. In comparison, ESP and DBS both have well defined strong force chains running through the centre of the specimens. These load bearing contact networks in these specimens are then supported by networks of weaker contacts orthogonal to the direction of the major principal stress. The large numbers of smaller circles on the left and right boundaries of the plots are indicative of this. Figure 6.7 visualises these weaker support contacts by plotting the bottom 25\textsuperscript{th} percentile of the contact force vectors.

At 15\% axial strain, the SPS still lacks the strong force chains that can be seen in the EPS and DBS.
Figure 6.5 Evolution of the contact force chains within each of the specimens (not scaled)
$\varepsilon_a = 5\%$ \hspace{1cm} $\varepsilon_a = 15\%$

Spherical Particle Specimen

Ellipsoidal Particle Specimen

DEM Ballast Specimen

Figure 6.6 Contact point distribution. The contact force vectors were filtered to 85th percentile.
Figure 6.7 Contact point distribution at 5\% strain. The contact force vectors were filtered to 25\% percentile
Figure 6.8 presents the contact normal fabric anisotropy analysed in terms of deviator fabric. The inherent anisotropy induced by the (identical) specimen preparation process is different and dependent on particle shape. The initial fabric seen with the EPS is slightly higher than DBS but not significantly. As previously seen in Chapter 3, shearing increases the intensity of the observed anisotropy. It can be seen that the increase in fabric anisotropy for the EPS and DBS is almost identical up to an axial strain of $\approx 2.3\%$. This correlates well with the similarity in volumetric behaviour seen between these two specimens up to the same strain, further supporting the suggestion that the effect of form is primarily dominant during the compression stage.

![Figure 6.8 Deviator fabric versus axial strain for spheres, ellipsoids and DEM ballast](image-url)
**Particle mechanics**

Particle rotation plays an important role in the dilatant and shear banding behaviour of granular media (Iwashita & Oda 1998). Figure 6.9 shows the frequency polygon of accumulated rotation experienced by the particles that make up the different specimens after 5% and 15% axial straining. The amount a particle rotates by is measured in degrees and the data is binned at 5° intervals. So for example after 5% axial strain, rotations of up to 5° were experienced by 19% of the particles in the SPS, 26% in the EPS and 46% of particles in the DBS. It can be observed that as many as 78% of the particles in DBS experienced up to 10° of rotation. On the other hand, 60% of particles in the EPS have an accumulated rotation of up to 10°. These low figures for particle rotation compared with the SPS are primarily because non-circular or non-spherical particles are capable of carrying moments that helps to resist rotation. The average particle rotation at 5% strain are 17.55°, 11.65° and 8° for the SPS, EPS and DBS respectively. After 15% axial strain, the average rotation for the SPS, EPS and DBS are 46.12°, 31.48° and 23.38° respectively. These observations confirm that particle rotation becomes less significant as particle geometry deviates away from a spherical shape.

Figure 6.10 shows the locations of all the particle centroids and the amount of rotation each particle has experienced. This is then overlaid by vectors that represent the displacement of the particle between 5 and 15% axial strain. It can be seen that a shear band develops in all specimens.
Figure 6.9 (A) Cumulative particle rotation at 5% axial strain. (B) Cumulative particle rotation at 15% axial strain.
Figure 6.10 Visulisation of cumulative particle rotation at 15% axial strain for Spheres (top), Ellipsoids (middle) and DEM ballast (bottom). The quivers represent particle displacement between 5 and 15% strain.
6.3. **Particle concavity and its effects**

In this section the mechanical significance of a concave particle shape is investigated using DEM.

The metric used to measure concavity is a modified version of the Fullness ratio as outlined by Mora and Kwan (2000) and is defined in 2D as,

\[
Concavity \text{ ratio (CR)} = \sqrt{\frac{\text{Concave area}}{\text{Area of particle}}}
\]

where the area of the a particle is measured from the projection on which the major and intermediate diameters of the particle lie. The concave area is defined as the area of the convex hull of the particle minus the area of the particle (Figure 6.11). A concavity ratio (CR) of zero will represent a particle that is perfectly convex (e.g. an ellipsoid) and as concavity moves away from zero the particle becomes increasingly more concave (Figure 6.12).

Concavity analyses of the Cliffe Hill (CH) and Glensanda (GS) ballast specimens are shown in Figure 6.13. While CH and GS both meet the industry specification for aggregates for the use as railway ballast, their CRs are very different. The ballast from CH is clearly concave to a greater extent than the GS specimen. It can be argued that greater concavity will improve the interlocking potential of a granular material and hence its ability to resist shear.

![Figure 6.11 Evaluation of the concave area from a particle's convex hull](image)

To investigate the mechanical effects of concavity, a potential particle was constructed that has a CR comparable to the median CR for the CH specimen.
(Figure 6.14). The form of the particle in terms of equancy \((S/L)\) is also comparable to the median equancy of the CH ballast. The angularity of the concave potential particle is 0.8682 and is effectively equivalent to the median angularity of 0.8588 for the Cliffe Hill ballast.

A numerical test specimen was prepared with particles having this shape and the same PSD (Figure 6.15) and modelling parameters as previous simulations (Table 6.2). An additional simulation was carried out using a specimen consisting of only one of the fourteen shapes (Chapter 4) in the DEM ballast mix. The chosen particle has an equancy \((S/L)\) ratio representative of the median equancy and angularity of the CH specimen. The tests were carried out at \(\sigma_3 = 200\) kPa. Results of the DBS simulation from the previous section are included here for comparison. Table 6.5 shows that both the initial void ratio and bulk density for the three different simulations are essentially the same and match well with void ratio measured from unsheared laboratory specimens using X-ray CT.

|                         | Void ratio | Bulk density  
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Single shape particle specimen (SSPS)</td>
<td>0.61</td>
<td>1.7081\times10^8</td>
</tr>
<tr>
<td>Concave particle specimen (CPS)</td>
<td>0.62</td>
<td>1.6844\times10^8</td>
</tr>
<tr>
<td>DEM ballast Specimen (DBS)</td>
<td>0.61</td>
<td>1.7078\times10^8</td>
</tr>
</tbody>
</table>
6. Modelling the effects of particle shape

Figure 6.12 Left: concavity = 0.112. Right: concavity = 0.305

Figure 6.13 Distribution of Concavity for the Cliffe Hill and Glensanada ballast

Figure 6.14 Exemplar concave DEM ballast constructed to match physical ballast
Figure 6.15 Internal slice taken from specimen made up of concave particles
6.3.1 Results

**Stress - strain behaviour**

Figure 6.16 presents the mobilised shear strength $\phi'_{mob}$ and volumetric strain $\varepsilon_{vol}$ against axial strain $\varepsilon_a$. The results clearly show that particle concavity positively affects the peak strength of a coarse granular material such as railway ballast (Table 6.6). The concave particle specimen (CPS) reached peak strength after an additional axial strain of 1.21% relative to the DBS simulation (Table 6.7). The volumetric response of CPS is also markedly different from that of the DBS even though their void ratio and bulk density are similar (Table 6.6). Figure 6.16 shows that the specimen of concave particles compresses less suggesting a stronger particle skeleton. This not only initiates volumetric expansion at a lower axial strain but also results in a rate of dilation almost double that of the DBS simulation. In contrast, the behaviour of the SSPS is remarkably similar to the DBS. Its peak mobilised effective friction angle is only slightly higher as a result of the slightly greater rate of dilation. However the critical state of the test does diverge away from the DBS and settles around 47°, similar to that of the concave specimen.

<table>
<thead>
<tr>
<th>Test no.</th>
<th>Ini. void ratio</th>
<th>Peak effective friction angle $\phi'_{peak}$ (°)</th>
<th>Max. volumetric strain (%)</th>
<th>Rate of dilation at $\phi'_{peak}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>SSPS</td>
<td>0.61</td>
<td>53.2675</td>
<td>0.7654</td>
<td>1.0238</td>
</tr>
<tr>
<td>CPS</td>
<td>0.62</td>
<td>57.4422</td>
<td>0.6656</td>
<td>1.5064</td>
</tr>
<tr>
<td>DBS</td>
<td>0.61</td>
<td>52.6555</td>
<td>0.8266</td>
<td>0.8029</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Test no.</th>
<th>$\varepsilon_a$ at $\phi_{peak}$ (%)</th>
<th>$\varepsilon_a$ at max. $\varepsilon_{vol}$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SSPS</td>
<td>6.3330</td>
<td>1.8327</td>
</tr>
<tr>
<td>CPS</td>
<td>7.3324</td>
<td>1.7471</td>
</tr>
<tr>
<td>DBS</td>
<td>6.1200</td>
<td>2.1634</td>
</tr>
</tbody>
</table>
Figure 6.16 The mobilised strength (A) and the volumetric strain (B) against axial strain.
Contact mechanics

Figure 6.17 presents the evolution of contact coordination number with respect to axial strain. At the start of shearing, $CN$ for the CPS was 9.07. This result is striking since contact coordination numbers of 7 and over have only previously been reported at much lower void ratios (e.g. Donev et al. 2004). A simple explanation for the higher $CN$ is that concavities increase the surface area of a particle thereby also increasing the number of contacts that are possible. X-ray CT analyses of laboratory triaxial test specimens (Chapter 2) have shown that $CN$ can be as high as 8.5. As all the particles in CPS simulation are of concave shape, the computed $CN$ is entirely plausible. As the specimen is sheared, the $CN$ initially rises due to compression and then rapidly reduces. A critical $CN$ is reached at around 6.2. This is equivalent to the initial $CN$ for both the SSPS and DBS.

![Graph showing the evolution of contact coordination number CN with axial strain](chart.png)

*Figure 6.17 Evolution of contacts coordination number CN with axial strain*
The similarity in stress-strain behaviour between SSPS and DBS seen previously is also observed in terms of $CN$. Both simulations have an initial $CN$ of $\approx 6$. The rate at which the number of contacts declines with shear is also comparable and $CN$ at the critical state is approximately 4.7 for both tests.

The spatial distribution of contact points, their magnitude and directionality are shown in Figure 6.18. At 5% axial strain, the SSPS and DBS simulations have similar force chains carrying similar loads. On the other hand, the higher $CN$ in the CPS equates to a better distribution of contact forces as load is transmitted through many more force chains which in turn reduces the average contact load. After an axial strain of 20%, the SSPS and DBS have very similar force networks where a few particles are taking on a disproportionately high load. The CPS of the other hand has a better distributed contact force network.

The fabric tensor analysis of the contact normal orientation is presented in Figure 6.19 in the form of deviator fabric vs axial strain. Particle concavity appears to have a modest effect on the intensity of contact normal anisotropy in a granular material.
Figure 6.18 Contact point distribution. The contact force vectors were filtered to 85th percentile.
Figure 6.19 Deviator fabric for concave particles

Particle mechanics

Figure 6.20 shows the frequency polygon of accumulated rotation experienced by the particles that make up the different specimens after 5% and 20% axial strain. The similarity between the SSPS and the DBS is evident at the particle level. Even though the distributions of cumulative rotation is (slightly) different, the average amounts of particle rotation experienced at 5% axial strain are comparable at 8.69° and 8° for the SSPS and DBS respectively. At 20% axial strain, average particle rotation remains comparable between the SSPS and DBS at 30.50° and 32.41° respectively. This variation is most likely caused by the difference in angularity range between the simulations; the DBS has a range of angularities and the less angular particles will rotate more, raising the average.

The CPS shows remarkably low levels of rotation at both strain levels. The average at 5% and 20% strain are 4.53° and 23.18° respectively. Figure 6.21 shows the locations of all the particle centroids and the amount of rotation each particle has experienced. This is then overlain by vectors that represent the displacement
of the particle between 5 and 20% axial strain. All three specimens develop shear bands. Particle rotation in the CPS is tightly concentrated at the shear band.
Figure 6.20 (A) Cumulative particle rotation at 5\% axial strain. (B) Cumulative particle rotation at 20\% axial strain.
Figure 6.21 Visulisation of cumulative particle rotation at 20% axial strain for SSPS (top), CSP (middle) and DBS (bottom). The quivers represent particle displacement between 5 and 20% strain.
6.4. Summary

The behaviour of granular media subjected to strain involves particle rearrangement and contact reorganisation. At lower void ratios, as in this case, rotation is inhibited by increased inter-particle contacts (i.e., increased $CN$). Therefore, energy applied during shear loading is consumed either in dilation to reduce the average number of contacts or in frictional slippage at contacts (Cho et al. 2006).

This chapter has investigated and assessed the effect of three independent particle shape parameters (form, angularity and concavity) using DEM. The novel aspect of this work has been the grounding of numerical shape parameters to measured values from real ballast material for the first time.

The stress-strain behaviour of coarse granular material such as railway ballast has been shown to change dramatically with changing particle shape. The simulations in Section 6.2 strongly suggest that, from a continuum perspective, changes in form and angularity manifest by altering the volumetric behaviour of a specimen. The results have shown that particles with non-unitary form (e.g. ellipsoids and DEM ballast) are able to pack more efficiently than particles with unitary form (e.g. spheres), thus exhibiting greater compression during initial stages of loading. Angularity, on the other hand, has been shown to influence the dilation characteristics of a granular medium by increasing the expansive rate of change of volume during shearing.

Contact coordination number $CN$ is known to be a function of particle shape and the results show that initially $CN$ increase with increased shape complexity. Once shearing starts, angular particles reveal the highest rate of contact slip. This finding justifies the previous conclusion that angularity increases dilatancy and explains the rapid loss of contacts during shearing compared with non-angular particles.

Particle shape fundamentally changes the way loads are transmitted through a granular medium and analyses of the contact force chains have shown that angularity facilitates the development of fewer but significantly stronger load
columns. This is a desirable trait in engineering applications where the available confinement of the granular mass is low such as a ballasted railway track.

Deviator fabric analysis of the contact normals has shown that all specimens are equally anisotropic indicating that the numerical specimen preparation method is effective. During loading, angular particles increase their directional preference more rapidly than the other particle shapes.

Measurements of cumulative particle rotation between 0-5% strain and 0-15% strain have shown that angularity is primarily responsible for impeding particle rotation.

The increase in shear strength due to particle concavity is modest compared with that of the other shape parameters and is brought on by a higher rate of dilation. This would suggest that concavity and angularity are of the same order of importance in the hierarchy of shape characteristics, although they measure different features.

While concavity greatly increases $CN$ as expected, it does not yield a proportional increase in shearing strength. Instead the stronger interlocking of the surrounding material constrains the shear band in a narrow zone limiting dilation and inducing critical state earlier.

Cumulative particle rotation measurements have shown concave particles to be highly resistant to rolling.

The behaviour of a specimen consisting of one unique particle shape (with mean form and angularity) compared to a specimen consisting of fourteen unique shapes is broadly similar. This proves to be an interesting result since it shows there is potential of capturing the behaviour of a specific granular medium through the use of a single, carefully designed DEM particle.
Final conclusions and future work

The work presented in this thesis has considered improvements to existing capabilities in modelling railway ballast and introduced new methods for the investigation of structure in large-scale granular specimens. A review of the pertinent literature reveals that modelling efforts have been hampered by a paucity of methods for the reliable assessment of fabric and a lack of real particle shape characterisation. A more accurate understanding of fabric in the ballast bed and improved parameterisation of numerical models will depend on the ability to observe structure in the ballast bed under field conditions and numerical reproduction of real particle shape.

Existing methods of direct observation of fabric [using XCT] are restricted to sands (i.e. in the sub-millimetre particle scale) that bear little relation to railway ballast which is typically an order-of-magnitude larger and much different in shape. While modelling using the Discrete Element Method offers the potential for investigating the effects of particle shape and its influence on the development of fabric, studies often give little justification for particle geometries that are chosen and in cases where realistic particle shapes are considered, the system scale and/or simulation time tend be unrealistic. To better understand the role and development of fabric in large granular systems such as a railway ballast bed, the ability to investigate both fabric and particle shape is important.
This thesis has considered the application of novel methods within the X-ray CT imaging, particle characterisation and DEM modelling domains.

In XCT imaging, new methods have been described for the imaging of preserved sections of railway ballast bed for the first time and the imaging of complete large triaxial test specimens (300 mm × Ø150 mm) at the μm scale was carried out for the first time. The large-scale imaging protocol used extended the specimen diameter range for granular media/geomechanics imaging to >250 mm with good spatial resolution, allowing the analysis of fabric that develop within the ballast bed at field and laboratory scale for the first time.

Void ratio analyses of whole triaxial test specimens showed that laboratory measurements of end-of-test \( e \) can vary by 12%, on average, from the XCT measurements and that homogeneity of prepared granular specimens can be difficult to achieve under laboratory conditions. The analysis of fabric in cyclically loaded triaxial test specimens and preserved field specimens from ballast beds has shown that initial particle orientation is highly anisotropic with more than 50% of the particles preferring an inclination of <30° to the horizontal. This remains largely unchanged after cyclic loading and stress reversal, primarily due to the confining stress inhibiting particle rotation. On the other hand the contact normal fabric is initially highly isotropic and cyclic loading has been shown to increase anisotropy by almost 50%. The results also showed that cyclic loading after a load reversal did not recover the state of anisotropy in the contact normal fabric that was present prior to stress rotation.

In the domain of particle characterisation, a simple and cost effective method for capturing three orthogonal images of particle was developed. The use of a green background in conjunction with a colour based segmentation algorithm has been shown to provide a robust, user invariant method of separating the ballast particle from the background. A new method of image-based diameter measurement is proposed. The algorithm fits geometric best-fit ellipses to the outline of the particles (iteratively) allowing it to better estimate the diameter.

Shape characterisation of ballast from two sources showed them to have quite different shapes even though they met the same Network Rail specification. This
is strong justification for the need to parameterise particle shape (in numerical modelling) thoroughly and unambiguously.

In the DEM modelling domain, a new protocol for the construction of realistic particle shapes has been put forward. This method follows a process where the parameterisation of shape is based on measured shape parameters of the ballast material being modelled. A new triaxial shear test model has been developed using the concept of potential particles that allows the use of realistic particle shape while keeping representative particle numbers and reasonable run times.

A parametric study is an important first step in validating a new numerical model. The analysis of the results showed that parameters associated with the modelling algorithm (timestep, shearing velocity/strain rate and damping) not only affects the response of the material but also adversely influence the efficiency of the model. It is therefore vital that appropriate values are chosen. The final calibrated model reproduced satisfactorily the overall response of scaled ballast in a monotonic triaxial shear test.

An investigation into the influence of particle shape parameters (form, angularity and concavity) was carried out using the calibrated DEM triaxial shear model. The results have shown that form, angularity and concavity affect the mechanical response of railway ballast differently under loading. Form enables the constituent particles of a granular mass to pack more closely allowing a strong interlocking fabric to develop. Angularity increases the number of contacts a particle is able to make while at the same time causes a faster rate of volume expansion which expedites contact slip during dilation. The effect of concavity was shown to be similar to that of angularity with the exception that its strongest mechanical effect is to impede particle rotation.

7.1. Future work

A number of final suggestions are made for work to follow or complement the developments and results set out in this thesis

- Characterising the shape of spent ballast would allow the quantification of realistic wear which can be different to classic abrasion tests. This
information could then be used to create DEM models to gain insight on how best to reuse recycled ballast safely.

- A method for *in situ* triaxial shear testing and simultaneous XCT imaging would be the natural step forward for the study of fabric in granular media. This would allow time resolved studies to be performed on the whole specimen.

- Evaluate the suitability of different specimen preparation methods (e.g. pluviation, pouring, etc.) using XCT.

- Automated method of particle geometry generation to expand the portfolio of DEM particles.

- Compare the differences in fabric response of ballast from different source.
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Appendices

A. X-radiation and imaging

X-rays are part of the electromagnetic waveform such as microwaves, visible light, and radio waves (Hsieh 2009). X-ray wavelengths $\lambda_{\text{wave}}$ can vary from $10^6$ µm to $10^{-3}$ µm and the energy $E_x$ of each photon of X-ray is proportional to its frequency and is described by

$$E_x = \frac{hc}{\lambda_{\text{wave}}} \quad (A.1)$$

where $h$ represents Planck’s constant (6.63×10^{-34} J-s), and $c$ the speed of light (3×10^8 m/s). Equation A.1 shows that the energy is proportional to its wavelengths and so as $\lambda$ get shorter the energy of the X-rays increases and as the wavelengths get longer the energy reduces. $E_x$ is measured in units of electron volts or eV and is equivalent to 1.6×10^{19} joules. X-rays with energy lower than 10 keV are considered as soft and since their penetration length is small and their use is limited to micron scale specimens. Hard X-rays ($E_x > 300$ keV) have large penetration lengths and are suited to large and high density specimens such as motor vehicle engine blocks. However it should be noted that with increasing energies the available contrast between phases reduces making analysis difficult.

X-rays are generated when high velocity free electrons are decelerated (by interacting with dense matter or change in trajectory) and any energy given up by the electron during the slowdown appears as electromagnetic energy known as X-radiation (Crouse et al. 2014). Free electrons (in industrial applications) are produced when a piece of conductive wire, often referred to as the filament, is energised by passing a current through it causing electrons to be freed due to thermal excitation as a result of the resistance in the wire. These negatively charged electrons are then accelerated by placing a positively charged metal (or anode) at close proximity to the filament (or cathode). Special target material (e.g. tungsten or copper) is usually embedded into the anode or placed between
the cathode and anode which gives the accelerated electrons a suitable material to interact with and produce X-rays (Figure a.1).

Three possible types of interaction can take place between the electrons and the target material producing.

- The electron approaches close to the nucleus of an atom and suffers a radiation loss, as shown in the upper-left part of Figure A.2. The line graph in Figure A.2 shows a typical X-ray spectrum produced by an X-ray tube operating at a 120-kV potential with additional filtration to remove the low-energy photons. The high-speed electron travels partially around the nucleus due to the attraction between the positive nucleus and the negative electron. The sudden deceleration of the electron produces bremsstrahlung radiation. The energy of the resulting radiation depends on the amount of incident kinetic energy that is given off during the interaction. If the energetic electron barely grazes the atomic coulomb field, the resulting X-ray has relatively low energy. As the amount of interaction increases, the resulting X-ray energy increases. This type of radiation is responsible for white radiation, which covers the entire range of the energy spectrum.

- A high-speed electron interacts with an inner-shell electron, which is then ejected from the atom, leaving an unoccupied lower energy level (the upper-middle part of Figure A.2 depicts a collision with a K-shell electron). This gap is filled by an outer-shell electron striving to the lowest energy position, and simultaneously a photon is released with an energy corresponding to the difference of energy levels of the two shells. Such photons take up only discrete energy values and are therefore called “characteristic radiation”.

- The third type of interaction occurs when an electron collides directly with a nucleus and its entire energy appears as bremsstrahlung. The X-ray energy produced by this interaction represents the upper energy limit in the X-ray spectrum. The probability of such collisions is low, as shown by its near-zero magnitude in the spectrum.
Figure A.1 Illustration of X-ray beam generation

Figure A.2 the different types of interaction that can take place between the electrons and the target material to produce X-rays (Hsieh 2009)

Figure A.3 The attenuation of X-ray photons (Crouse et al. 2014)
A.1. Interaction of X-rays with matter

When X-rays are directed into an object, some of the photons (or packets of X-ray energy) interact with the particles of the matter and their energy can be absorbed or scattered (Figure A.3). This absorption and scattering is called attenuation. Other photons travel completely through the object without interacting with any of the material’s particles. The number of photons transmitted through a material depends on the thickness, density and atomic number Z of the material, and the energy of the individual photons.

The total attenuation is the sum of the attenuation due to different types of absorption and scatter interactions. The type of interaction that occurs is dependent on the material and X-ray energy used. For geotechnical applications, the photoelectric effect (PE) is the dominant attenuation mechanism at low X-ray energies, up to approximately 50–100 keV. For energies up to 500 – 1000 keV Compton scatter (C) is dominant. This is illustrated in Figure A.4.

Photoelectric absorption (illustrated in Figure A.5) of X-rays occurs when the X-ray photon is absorbed, resulting in the ejection of electrons from the outer shell of the atom, and hence the ionization of the atom. Subsequently, the ionized atom returns to the neutral state with the emission of an X-ray characteristic of the atom. This subsequent emission of lower energy photons is generally absorbed and does not contribute to (or hinder) the image making process. Photoelectron absorption is the dominant process for X-ray absorption up to energies of about 500 keV. Photoelectron absorption is also dominant for materials of high atomic numbers.

Compton scattering (illustrated in Figure A.5b) occurs when the incident X-ray photon is deflected from its original path by an interaction with an electron. The electron gains energy and is ejected from its orbital position. The X-ray photon loses energy due to the interaction but continues to travel through the material along an altered path. Since the scattered X-ray photon has less energy, it, therefore, has a longer wavelength than the incident photon. The event is also known as incoherent scattering because the photon energy change resulting from
an interaction is not always orderly and consistent. The energy shift depends on
the angle of scattering and not on the nature of the scattering medium.

**X-ray attenuation**

The absorption of a monochromatic X-ray beam with intensity $I$ propagating
through a homogeneous material with respect to the traversed distance is
described by the law of Beer-Lambert. The change in X-ray beam intensity at
some distance $x$ in a material can be expressed in the form

$$dl(x) = -I(x) \cdot \sigma_a \cdot n_z \cdot dx$$  \hspace{1cm} (A.2)

where $n_z$ is the number of atoms/cm$^3$, $d_z$ is the incremental thickness of material
traversed and $\sigma_a$ is a proportionality constant that reflects the total probability
of a photon being scattered or absorbed. Integrating Equation A.1 gives,

$$I = I_0 e^{-\sigma_a n_z x}$$  \hspace{1cm} (A.3)

Combining $n_z$ and $\sigma_a$ yield a material specific constant usually referred to as the
linear attenuation coefficient $\mu$. Therefore the equation becomes:

$$I = I_0 e^{-\mu x}$$  \hspace{1cm} (A.4)

When the X-rays are traveling through inhomogeneous matter, Equation A.4 is
becomes,

$$I = I_0 e^{\sum \sigma(z_i) x_i}$$  \hspace{1cm} (A.5)

where each increment $i$ corresponds to a single material with attenuation
coefficient $\mu_i$ over a linear extent $x_i$. In general, X-ray beams are not
monochromatic and the linear attenuation coefficients depend on the ray energy
$E_x$. Consequently, formula Equation A.5 has to be adapted for polychromatic X-
rays such that,
Appendix

\[ I = I_0(E_x)e^{\sum(-\mu_i(E_x)x_i)dE_x} \quad (3.6) \]

However, such a calculation is usually problematical for industrial CT, as the precise form of the X-ray spectrum, and its variation at off-centre angles in a fan or cone beam, is usually only estimated theoretically rather than measured. As a result commonly used reconstruction algorithms can only solve Equation A.4 and so the variations in the X-ray energy spectrum can cause imaging artefacts.

![Figure A.4](image)

*Figure A.4 The attenuation due to different types of absorption and scatter interactions*

(a) Photo-electric effect  
(b) Compton scattering

*Figure A.5 (a) Photo-electric absorption is dominant between 50 – 100 keV (b) Compton scatter is dominant up to 500-1000 keV.*

A.2. X-ray detection

For the purposes for imaging, X-ray detectors (e.g. film or electronic CCDs) effectively count the number of photons that pass through the object along a certain ray-path. Modern X-ray CT systems use electronic detectors to convert these incoming attenuated X-ray radiation into an electric (digital) projection signal which is then reconstructed to a 2-D or 3-D distribution of local object attenuation values.

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Integrated scintillation detectors are the current state-of-the-art technology for medical and industrial CT systems. Incoming X-rays are first absorbed by the scintillation crystal and emitted as visible light. The visible light is then detected by the photodiode layer and converted into an electrical signal. Common scintillator materials are cesium iodide, gadolinium oxysulfide, and sodium metatungstate. Each pixel on the detector has a crystal above it and space between individual crystal/pixel combination are filled with a highly reflective material like titanium dioxide (TiO₂) that prevents optical light from entering the scintillator crystal that corresponds to another pixel (Figure A.6). The electrical current from the photodiode is integrated over a given amount of time. At the end of the integration period, the resulting charge is read-out and the next integration period starts. The read-outs are passed to a computer for conversion into digital radiographs or sinograms depending on the beam/detector geometry used.

A.3. X-ray beam geometries

Figure A.7 illustrates some of the most common beam configurations in CT scanners. In fan/planar beam scanning, X-rays are collimated and measured using a linear detector array. Typically, slice thickness is determined by the aperture of the linear detector array. Collimation is necessary to reduce the influence of X-ray scatter, which results in spurious additional X-rays reaching the detector from locations not along the source-detector path. Linear arrays can generally be configured to be more efficient than flat panel detectors, but have the drawback that they only acquire data for one slice image at a time (Ketcham 2012).

In cone-beam scanning, the linear array is replaced by a flat-panel (or planar) detector, and the beam is no longer collimated. Data for an entire object, or a considerable thickness of it, can be acquired in a single rotation. The data are reconstructed into images using a cone-beam algorithm. In general, cone-beam data are subject to some blurring and distortion the further one goes from the central plane that would correspond to single-slice acquisition. They are also more subject to artefacts stemming from scattering if high-energy X-rays are utilized. However, the advantage of obtaining data for hundreds or thousands of slices at
a time is considerable, as more acquisition time can be spent at each turntable position, decreasing image noise.

Parallel-beam scanning is done using a specially configured synchrotron beam line as the X-ray source. In this case, volumetric data are acquired and there is no distortion. However, the object size is limited by the width of the X-ray beam; depending on beam line configuration, objects up to 6 cm in diameter may be imaged. Synchrotron radiation generally has very high intensity, allowing data to be acquired quickly, but the X-rays are generally low-energy (< 35 keV), make dense materials difficult to image.
Figure A.6 Schematic of typical anatomy of XCT scanner detector. Collimators guide the beams of attenuated X-ray and the scintillators convert X-rays into visible light for detection.

Figure A.7 Illustration of beam geometries (Ketcham 2012)
B. Modelling the membrane

Many published DEM simulations of element tests have used rigid walls as the test boundaries in combination with a servo controlled system to control the stresses (e.g. Cheng et al. (2004)). In contrast, Thornton (2000) and Lin and Ng (1997), amongst others, simulated triaxial test stress conditions using a periodic cell. In comparison with periodic boundaries, specimens bounded by rigid walls are a closer approximation to laboratory element tests. The lateral boundary of laboratory triaxial test specimens is formed by a flexible latex membrane that allows the pressure within the triaxial cell to be transferred to the specimen; at the same time no constraint is imposed upon lateral deformation. The specimen can bulge and localizations or shear bands can form. Where a test is simulated using rigid boundaries, while the overall stress state can be attained using the servo-controlled approach (discussed in Section 5.2.3), the rigid walls may inhibit the development of these localizations and there may be significant non-uniformities in the stresses applied along the boundary.

Instead of modelling an elastic membrane in a DEM analysis, the essential function of the membrane (which is to apply a confining pressure to the exterior of the specimen), may be simulated by constructing a triangular mesh between the centroids of particles deemed to be on the surface of the specimen. The confining force on each triangle is calculated as the product of the confining pressure and the area of the triangle and this force is distributed to the particles in proportion to the relative cross-sectional areas of their circumscribing spheres.

Consideration must be given to the interface between the cylindrical part of the specimen and the edge of the platen. In a real triaxial cell, the elastic membrane ends at the end of the platens. This is simulated by introducing a circular ring of nodes on the top and bottom platens which become part of the mesh. The radii of these rings are set by calculating the effective radius of the surface particles adjacent to the top and bottom platens. If the specimen expands laterally adjacent to the platens during the test, the radius of the ring of virtual particles can either remain fixed or be altered to match this movement.
**Surface mesh construction**

If the centroids of the particles in a specimen are considered as a cloud of points, an outer surface can be defined consisting of a triangular mesh (with nodes at the centroids of the particles) which wraps around the outside of the cloud. One method of identifying a surface mesh is to look at the network formed by the contacts between these surface particles and then find a contiguous mesh of triangles on the surface. In this case, a different approach was adopted that makes use of the computational geometry library CGAL (www.cgal.org). First, a Delaunay triangulation is performed over all the particle centroids. The surface mesh is then found as a subset of the Delaunay triangulation, called an alpha shape as described below.

For a set $P$ of points in 3-dimensional Euclidean space, the Delaunay triangulation is a triangulation $DT(P)$ such that no point in $P$ is inside the circumscribing sphere $S_i$ of any tetrahedron in $DT(P)$. In 3 dimensions, the triangulation refers to the subdivision of the space into tetrahedra, whose vertices are the points $P$. For a 3-dimensional point cloud the outer surface of this Delaunay triangulation will be a mesh of triangles formed from the tetrahedral faces that have no adjacent tetrahedral. This triangle mesh will always form a convex polyhedron that encloses the point cloud as if a thin elastic sheet were stretched over the cloud of points. For the purposes of transferring a confining pressure to the outer particles, this mesh is not useable as it does not (generally) enclose the shape of the cloud tightly. It is a question of defining which points are outer points. This is illustrated with the 2-dimensional Delaunay triangulation depicted in Figure B.1. In two dimensions, no point can be inside the circumscribing circle of any triangle. Figure 5.7 (a) shows the Delaunay triangulation of a small cloud of points in $\mathbb{R}^2$. It can be seen that the perimeter of the triangulation does not include points A and B. In the context of a virtual membrane, this would mean that the particles corresponding to points A and B would not be subjected to a confinement force. In order to include A and B in the perimeter, it is necessary to prune away some of the outer Delaunay triangles – in this case, triangles A and B in Figure B.1 (b). The mechanism for achieving this is to limit the maximum radius of a triangle’s circumscribing circle. For the outer triangles of a triangulation, the
circumscribing circles can be very large as there are no points to get in the way, as illustrated by the circumscribing circles for triangles A and B.

Figure B.1 Example of alpha shape formation for 2-dimensional point cloud

By limiting the maximum permissible circle radius, these surface triangles can be removed from the triangulation, leaving a surface which conforms more closely to the ‘shape’ of the point cloud as shown in Figure B.1 (c). The extension of this principle to 3D involves limiting the maximum radius of a tetrahedron’s circumscribing sphere, $S_i$. This is performed in the CGAL library via the parameter $\alpha = (maximum\ sphere\ radius)^2$. The effect of varying $\alpha$ on the triangulation of a triaxial specimen can be seen in Figure B.2. As the shape of a point cloud is a rather vague notion, obtaining a suitable fit requires some human input in the selection of $\alpha$. If $\alpha$ is too large, then some of the surface particles will be missed out. On the other hand, if it is too small, the triangulation can penetrate into the body of the point cloud (or even form isolated internal pockets). This latter case would clearly lead to undesirable behaviour, but in practice it is relatively easy to choose a suitable (and safe) value for $\alpha$. The method for tuning alpha, which was performed only once and used in all of the subsequent simulations, is simply to start with a large value and reduce it until all of the clearly visible surface particles are included in the membrane. The chosen value was $\alpha = (maximum\ particle\ radius \times 1.5)^2$. Because the model consists of a
relatively dense assembly of particles, in practice the problem of virtual membrane penetration does not occur.

\[ \alpha = \left( \text{maximum particle radius} \times 1.5 \right)^2 \]

*Figure B.3 Sequence of alpha shapes with parameter $\alpha$ reducing from top left ($\alpha = \infty$) to bottom right $\alpha = (\text{maximum particle radius} \times 1.5)^2$*

**C. Volume measurement in DEM**

Two approaches were used to calculate the void ratio; a computationally fast method involving a small approximation, performed during the simulation, and a very accurate but slower method which could be used during post-processing for selected states. For very accurate measurements, a three-dimensional scan of a region within the specimen was made. The region was subdivided into a rectangular array of voxels and each point tested for inclusion within a particle. The void ratio could then be determined from these data. The fast method involved calculating the volume of the polyhedron formed by the virtual membrane and platens, calculated as the sum of the signed (+ive or -ive) volume of tetrahedra formed from a common reference point and each triangle of the polyhedron. The solid volume contained within this polyhedron was approximated as the sum of the volumes of the internal particles added to half of the volume of the surface particles. The void ratios presented in the graphical results were calculated using this method.
D. Matlab programs

D.1. Ellipse fitting

```matlab
%% count no. of files to be processed
directory = 'X:\Particle_characterisation\Glen_sanders\X\';
tifFiles = dir([sdirectory '*' '.tif']);
n=length(tifFiles);

%% create cell array to hold results.
mat = ones(n+1,17); % add 1 extra row for label
zres = cell(size(mat));

zres(1,1:17) = {'ID', 'a', 'b', 'angle', 'x0', 'y0', 'no. of obj.', 'area of obj.', 'area of ellipse', 'Major Axis Length', 'Minor Axis Length', 'obj.peri.', 'B_a', 'B_b', 'B_angle', 'B_x0', 'B_y0'}; %labels the table.

%% estimate particle dimension using ellipse fitting
for i=1:n;
    filename = [sdirectory tifFiles(i).name];
    img = imread(filename);
    img = rgb2gray(img); % convert image to grayscale

    % Convert to binary and remove small artifacts
    img = img>10;
    img = bwareaopen(img,1000);

    %count no. of obj in img
    count = bwconncomp(img);

    % object parameters
    stats = regionprops
        (img,'Area','MajorAxisLength','MinorAxisLength','Perimeter','BoundingBox');
    bou_a = [stats(:).BoundingBox(4)];
    bou_b = [stats(:).BoundingBox(3)];

    % find boundary
    boun = bwboundaries(img);
    xy = boun(1); % x&y coordinates of the boundary
    xy = xy';

    [zb, ab, bb, alphab] = fitellipse(xy, 'linear'); %algebraic ellipse fitting
    [zg, ag, bg, alphag] = fitellipse(xy); %geometric ellipse fitting

    % pack results into cell array
    zres(i+1,1)={'tifFiles(i).name'};
    zres(i+1,2)={max(ag, bg)};
    zres(i+1,3)={min(ag, bg)};
    zres(i+1,4)={alphag};
    zres(i+1,5)={zg(1)};
    zres(i+1,6)={zg(2)};
    zres(i+1,7)={count.NumObjects};
    zres(i+1,8)={stats(:).Area};
    zres(i+1,9)={pi*ag*bg};
    zres(i+1,10)={max(bou_a,bou_b)};
end
```
zres(i+1,11) = {min(bou_a,bou_b)};
zres(i+1,12) = {{stats(:,).Perimeter}};
zres(i+1,13) = {max(ab, bb)};
zres(i+1,14) = {min(ab, bb)};
zres(i+1,15) = {alphab};
zres(i+1,16) = {zb(1)};
zres(i+1,17) = {zb(2)};

end

D.2. Contact plane fitting

%% separates disconnected pieces inside a patch defined by faces (F) and vertices (V). CLU is a structure array with fields "faces" and "vertices". Each element of this array indicates a separately connected patch. X holds the count of faces for each element in CLU.
% DO Not run if data already split [clu,x] = splitFV(surface);

%% filter out small patch based on no of faces e.g. 1 voxel will have 4 faces.
id = x>0;
contacts = clu(id);

%% initialise output variables
[n, m] = size(contacts);  % holds the angle between normal and 'z'
pc_rads = zeros(n,1);      % (0 0 1) using 'princomp'
pc_normal = zeros(n,3);
pc_fitted = repmat(struct('Xfit',[],'Yfit',[],'Zfit',[]), n, 1);  % holds the normal vectors using 'princomp'

%% perform PCA on each element in contacts
for i=1:n;
data = contacts(i,1).vertices;

%% Fit plane using Principal component analysis (PCA)
[coeff, score, roots] = pca(data);

%% Get unit normal of fitted plane
pc_normal(i,:) = coeff(:,3)';  % fill with normal vector 'row = ID'

%% [m,p] = size(data);
meanX = mean(data,1);
fitted = repmat(meanX,m,1) + score(:,1:2)*coeff(:,1:2)';
pc_fitted(i,1).Xfit = fitted(:,1);
pc_fitted(i,1).Yfit = fitted(:,2);
pc_fitted(i,1).Zfit = fitted(:,3);

%% calculate direction cosine from Z (vertical) axis
pc_rads(i,1) = acos(dot(pc_normal(i,:), [0 0 1]));
end
clear('n', 'i', 'data', 'm', 'coeff', 'score', 'roots', 'normal')

D.3. Fabric tensor

%% carry out tensoral multiplication to calculate fabric tensor
C = [x,y,z]; % x,y&z are the contact plane normal vector

var = 0;
f_mat = zeros(3,3);
fabric_tensor = zeros(3,3);
[n,m] = size(C);
cc = 1;
for ii=1:3
  for jj=1:3
    for s=1:n
      var(s,cc) = C(s,ii)*C(s,jj);
    end
    cc=cc+1;
  end
end

%%
%   Nii  Nij  Nik
%   Nji  Njj  Njk
%   Nki  Nkj  Nkk

f_mat(1,1) = sum(var(:,1));   % Nii
f_mat(1,2) = sum(var(:,2));   % Nij
f_mat(1,3) = sum(var(:,3));   % Nik

f_mat(2,1) = sum(var(:,4));   % Nji
f_mat(2,2) = sum(var(:,5));   % Njj
f_mat(2,3) = sum(var(:,6));   % Njk

f_mat(3,1) = sum(var(:,7));   % Nki
f_mat(3,2) = sum(var(:,8));   % Nkj
f_mat(3,3) = sum(var(:,9));   % Nkk

%%
fabric_tensor = f_mat/n
[eigen_vec, eigen_val] = eig(fabric_tensor); % solve eigen value problem

clear('jj', 'ii', 'cc', 'n', 'm', 'C', 'var', 's')