Mesoscopic Modelling of Concrete Using a Bonded Discrete Element Method

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Declaration

I, Anthony Wang, declare that the work contained in this thesis has not been submitted for any other degree or professional qualification. With the exception of the raw simulation data used for the results presented in Chapter 3, which were obtained by means of a collective research effort between Ron Kou, Artur Szlachetka, and myself; all results, discussions, and conclusions represent my own work, carried out under the supervision of Professor Jin Y. Ooi between September 2017 and April 2018. Where other sources are quoted full references are given.

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Abstract

Concrete’s key mesoscopic strength, stiffness, and damage descriptors are identified, examined, and quantitatively related to essential bulk behavioural properties by means of a comprehensive parametric investigation of numerically-simulated displacement-controlled uniaxial compression tests using an existing bonded discrete element model (Edinburgh Bonded Particle Model). Results demonstrate that the mesoscopic tensile-to-shear ratios of stiffness and strength are closely linked and fundamentally related to concrete’s bulk elastic and failure behaviour. Specifically, analysis of mechanical phenomena at the mesoscale revealed that a proportional relationship exists between mesoscopic tensile-to-shear stiffness and bulk compressive strength by virtue of a macroscopic Poisson effect. In addition, evaluation of DEM-computed ultimate compressive strength using newly proposed calibration equations shows strong quantitative agreement for all numerical specimens tested. As such, the importance of selecting mesoscopic mechanical parameters based on their collective impact, rather than based on the sum of their direct individual effects, is emphasised. Lastly, a full set of results concerning the model’s geometrical and contact friction input parameters showed that the model is able to capture various scaling and boundary-confinement features consistent with experimental studies from other sources. These results also showed that bond fabric properties such as bond coordination number and porosity are closely correlated to DEM-computed bulk results, indicating that fabric properties can be used as effective bulk calibration parameters.
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Nomenclature

Roman characters

\( A \) \hspace{0.5cm} \text{Cross-sectional area} \\
\( A_S \) \hspace{0.5cm} \text{Shear bulk strength coefficient} \\
\( A_T \) \hspace{0.5cm} \text{Tensile bulk strength coefficient} \\
\( B \) \hspace{0.5cm} \text{Number of bonds} \\
\( B_b \) \hspace{0.5cm} \text{Bond breakage at peak stress} \\
\( b_d \) \hspace{0.5cm} \text{Damping ratio} \\
\( C \) \hspace{0.5cm} \text{Fabric coordination number} \\
\( C_S \) \hspace{0.5cm} \text{Shear contribution coefficient} \\
\( C_T \) \hspace{0.5cm} \text{Tensile contribution coefficient} \\
\( d \) \hspace{0.5cm} \text{Displacement} \\
\( D \) \hspace{0.5cm} \text{Specimen diameter} \\
\( D_m \) \hspace{0.5cm} \text{Local damage} \\
\( e \) \hspace{0.5cm} \text{Coefficient of restitution} \\
\( E \) \hspace{0.5cm} \text{Young’s modulus} \\
\( E_{c(0.4)} \) \hspace{0.5cm} \text{Bulk Young’s modulus} \\
\( E_r \) \hspace{0.5cm} \text{Relative error} \\
\( E^* \) \hspace{0.5cm} \text{Equivalent Young's modulus} \\
\( f_c' \) \hspace{0.5cm} \text{Ultimate cylinder compressive strength} \\
\( f_s \) \hspace{0.5cm} \text{Shear factor} \\
\( F \) \hspace{0.5cm} \text{Force} \\
\( G \) \hspace{0.5cm} \text{Shear modulus} \\
\( h \) \hspace{0.5cm} \text{Height of specimen} \\
\( I \) \hspace{0.5cm} \text{Second moment of area} \\
\( K \) \hspace{0.5cm} \text{Stiffness matrix}
\( k_n \)  Bond normal stiffness
\( k_s \)  Bond shear stiffness
\( L_b \)  Bond length
\( L_r \)  Loading rate
\( m \)  Particle mass
\( m^* \)  Equivalent particle mass
\( M \)  Bending moment
\( n \)  Porosity
\( P \)  Number of particles
\( r \)  Particle radius
\( r_b \)  Bond radius
\( r_c \)  Contact radius
\( S_n \)  Hertz-Mindlin normal stiffness
\( S_t \)  Hertz-Mindlin tangential stiffness
\( S_C \)  Mean bond compressive strength
\( S_S \)  Mean bond shear strength
\( S_T \)  Mean bond tensile strength
\( u \)  Displacement vector
\( V \)  Velocity
\( V^* \)  Equivalent velocity
\( Z \)  Position of loading plate

Greek characters
\( \alpha \)  Tensile-to-shear bond strength ratio
\( \beta \)  Reduction factor
\( \delta \)  Overlap
\( \Delta t \)  Time step
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>$\Delta t_{\text{crit}}$</td>
<td>Critical time step</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>Bulk axial strain</td>
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<tr>
<td>$\varepsilon_c$</td>
<td>Bulk strain at peak compressive stress</td>
</tr>
<tr>
<td>$\varepsilon_r$</td>
<td>Bulk radial strain</td>
</tr>
<tr>
<td>$\eta$</td>
<td>Contact radius multiplier</td>
</tr>
<tr>
<td>$\iota_d$</td>
<td>Global damping coefficient</td>
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<tr>
<td>$\kappa$</td>
<td>Shear correction coefficient</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>Bond radius multiplier</td>
</tr>
<tr>
<td>$\mu_s$</td>
<td>Coefficient of static friction</td>
</tr>
<tr>
<td>$\mu_r$</td>
<td>Coefficient of rolling friction</td>
</tr>
<tr>
<td>$\nu$</td>
<td>Poisson’s ratio</td>
</tr>
<tr>
<td>$\nu_{c(0.4)}$</td>
<td>Bulk Poisson’s ratio</td>
</tr>
<tr>
<td>$\xi$</td>
<td>Radius ratio</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Density</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Stress</td>
</tr>
<tr>
<td>$\sigma_c$</td>
<td>Bond compressive strength</td>
</tr>
<tr>
<td>$\sigma_s$</td>
<td>Bond shear strength</td>
</tr>
<tr>
<td>$\sigma_t$</td>
<td>Bond tensile strength</td>
</tr>
<tr>
<td>$\zeta$</td>
<td>Coefficient of variation</td>
</tr>
<tr>
<td>$\phi$</td>
<td>Timoshenko shear coefficient</td>
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Chapter 1   Introduction

1.1   Background

With over 4.5 billion metric tonnes of ready-mix concrete produced annually and a global market size valued at over $500B (GVR, 2016), concrete is at present the most commonly used building material in the world. Due to its essential role in today’s infrastructure and construction-driven environment, and with the rapid innovation of new mixes (e.g. high-performance concrete) and technologies (e.g. 3D concrete printing), there is a persistent need for methods to study and predict the performance of this material.

1.2   Literature review

1.2.1   Computational methods for modelling of concrete

The literature proposes countless methods to study and analyse concrete behaviour. Amongst these, some of the most widely-used are computational methods. These techniques possess certain advantages when compared to analytical and experimental methods. First of all, computational modelling offers the possibility to directly extract internal forces and displacements at any stage of the simulation, without the need to assume these based on measured boundary data. In addition, these methods are easily adapted to account for different loading configurations, boundary conditions, and material properties (Cundall & Strack, 1979). Finally, as computational power and capacity continue to improve with time, computer simulations are increasingly expected to replace their, often much costlier, experimental counterparts in the research and development stage of many engineering applications.

1.2.1.1   Continuum-based methods

From a numerical standpoint, modelling of concrete can be classified into two branches of methods: those where the solid is represented as a continuum and those where it is represented as a discrete medium. Continuum-based approaches, such as the Finite Element Method (FEM), are widely used in conventional structural engineering practice, however, their application in modelling fracture behaviour at
the microscopic level remains limited. Whilst extensions to classical continuum-based methods have been developed to allow for the possibility of crack modelling, e.g. the eXtended Finite Element Method (XFEM) (Moës, et al., 1999), these approaches are ill-suited to model multiple fractures with joining and bifurcating cracks (Leclerc, 2017). Similarly, other continuum-based methods developed to study cracking phenomena require additional means such as remeshing of lattices (Kim & Buttlar, 2009) or making a-priori assumptions regarding crack path location (Bažant, 2002). To summarise, the complex constitutive behaviour of concrete, arising from extensive micro- and macro-cracking, remains challenging to characterise in terms of a continuum formulation (Burlion, et al., 2000). Whereas continuum-based methods are certainly indispensable for solving traditional (structural) engineering problems, their wide applicability in that respect does not strictly translate to their suitability for studying problems where microscopic discontinuities, such as crack initiation and propagation, are of primary importance.

1.2.1.2 Discrete methods

In contrast to continuum-based approaches, discrete methods have the advantage that they inherently reproduce the discontinuous nature of the material (Donzé, et al., 2008), making them ideal for mechanical problems where multiple scales and discontinuities exist. One such discrete method showing good promise in the field of concrete modelling is the Discrete Element Method (DEM).

Originally created by Cundall (1971) to tackle problems in the field of rock mechanics, the DEM consists of a family of numerical techniques whereby an explicit numerical time-stepping scheme is used to model the dynamic interactions of a finite number of independent, rigid particles (discrete elements). The DEM fundamentally differs from continuum-based methods in that the kinematic and equilibrium relations used in continuum analysis are replaced by Newton’s equations of motion applied to each individual particle. As such, the material’s constitutive relation is moved from the macroscopic scale to the particle level and takes the form of contact laws (Potyondy & Cundall, 2004).

The underlying assumption of the DEM is that the mechanical behaviour at the bulk level can be approximated by considering the collective effect of particles at
the microscopic level, each undergoing individual loading and unloading processes, sliding effects, and displacements (Tran, et al., 2011). For this reason, the most crucial part of any DEM is the contact law describing how particles interact and the way in which these interactions affect bulk behaviour (Kuhl, et al., 2000). Currently, the two main disadvantages of the DEM are the increased computational cost, and the necessity of a complex and time-consuming macro-micro calibration procedure (Hentz, et al., 2004a).

In conclusion, both modelling approaches, each with its own set of inherent strengths and weaknesses, have their place in the current landscape of concrete fracture modelling. A recent study by Skarżyński, et al. (2015) in which both methods were directly compared with experimental tests and μCT images summarised these strengths and weaknesses concisely by concluding the following: “FEM results are more accurate as compared with experiments since the calibration procedure is based on macro-scale properties... [In contrast], DEM better follows the fracture processes such as the onset, formation and propagation of micro- and macro-cracks. In addition, DEM allows for a more detailed investigation of different microstructural phenomena which affect the macroscopic behaviour”.

1.2.2 Discrete mesoscopic representation of concrete

According to Wang, et al. (2016), the term ‘mesoscale’ is traditionally defined as the largest length-scale with observable heterogeneity. In relation to concrete, most studies in the literature propose that the mesostructure of concrete contains voids, aggregates, mortar and interfacial transition zones (ITZ) (Zhou, et al., 2017; Suchorzewski, et al., 2018; Murali & Deb, 2018). A wide range of models and methods have been used by researchers to represent concrete at this length-scale; each possesses some form of each of the following components:

i) Initial particle packing: the initial assembly of particles representative of the physical substance that makes up a concrete specimen;

ii) Contact law: the constitutive relationships at the mesoscopic level describing contact force-displacement behaviour;
iii) **Damage law and failure criteria:** the failure criteria which represent the propagation of cracks and the gradual development of damage inside a specimen in response to load;

### 1.2.2.1 Initial particle packing

“The generation of a suitable initial configuration is the first step of every DEM simulation” (Ergenzinger, et al., 2011).

The literature reports two main schools of thought concerning the creation of initial particle packings. The first approach considers concrete as a single-phase material whereby all particles and bonds in the system have the same material properties (Tran, et al., 2011; Brown, et al., 2014). This approach naturally requires fewer discrete elements and meso-parameters, thus offering a simpler calibration procedure in addition to being less computationally demanding compared to its multi-phase counterpart. The second approach considers concrete as a multi-phase material where aggregates, cement mortars, and in some cases, even the interfacial transition zones are each represented separately. Whilst not as popular initially, thanks in part to advances in computing power, this method has gained prominence and has often been used in combination with experimental methods such as aggregate sieve analysis (Sinnaie, 2017) and X-ray computed tomography (Suchorzewski, et al., 2018) to create specimens which are consistent with laboratory tests.

Although the multi-phase approach provides a higher resolution for analysis and offers insight into the complex interactions between the various mesoscopic phases of concrete as showcased by Murali & Deb (2018), computational cost remains a challenge. On the topic of DEM modelling of concrete using multiple phases, Skarżyński et al. (2015) state: “The disadvantages [of multi-phase DEM] are: enormous computational cost and a difficult calibration procedure...” To illustrate, the DEM computation time of a single $50 \times 50 \times 50$ mm$^3$ cube consisting of 325,000 spherical particles studied by Suchorzeski, et al. (2018) took 14 days using a PC with CPU 2.8 GHz. In comparison, 3D single-phase models reported in the literature generally do not exceed 30,000 particles, regardless of specimen size (Brown, et al., 2014; Tran, et al., 2011; Oñate, et al., 2015). Given these constraints, the multi-phase
1.2 Literature review

approach, while interesting for pure research purposes, remains limited in its applicability to real engineering situations. As such, if the aim is to develop DEM models able to simulate realistic, large-scale structures, the single-phase approach remains more suitable.

1.2.2.2 Contact law

The contact law of a DEM model can be seen as the formulation of the material model on the microscopic level (Labra, 2012). Whereas conventional DEM contact laws describe the interactions of cohesionless particles, contact laws designed for the simulation of cementitious materials incorporate the effects of cementation by bonding particles with each other such that the contacts are able to resist tensile forces.

Most approaches developed to represent the cement mechanism fall within one of two categories; contact-bond models, or beam-bond models. The first of these considers particles to be bonded by a pair of elastic springs with normal and shear stiffnesses acting at the point of contact (Cho, et al., 2007). As these connections are unable to carry bending moments, previous studies that used this method to model concrete have either implemented an artificial rotational stiffness term (Sinnaie, 2017; Tran, et al., 2011) or neglected the moment calculation altogether by making the crude assumption that the effect of bending moments is negligible compared to other internal forces (Nitka & Tejchman, 2015). Unlike contact-bond models, beam-bond models use beam elements which comprise a link between the centres of two bonded particles. When using beams, the elastic behaviour can be based on Euler-Bernoulli (André, et al., 2012) (Leclerc, 2017) or Timoshenko (Obermayr, et al., 2012) (Brown, et al., 2014) beam theory. In these cases, the elements are able to resist tensile forces, moments, and in the case of Timoshenko beams, shear forces.

In addition to a bonded component, contact laws designed to model concrete must also include a non-bonded component to describe the contacts which occur between uncemented particles as a result of bonds breaking or when two new particles come into contact. These non-bonded contacts, although an integral part of the DEM model, do not have a significant contribution towards the strength and stiffness of a specimen (Sinnaie, 2017) and are almost unanimously represented by
traditional cohesionless contact laws such as linear elastic or Hertz-Mindlin contact models.

1.2.2.3 Damage law and bond failure criteria

As hinted at previously, bonded contact models for concrete require a method through which inter-particle bonds can fail. This failure represents the fracture and progressive deterioration in the specimen (Brown, 2013). Most damage models presented in the literature compare the state of each bond at every time step to a predefined set of bond failure criteria. In the case of contact-bond models, these criteria are often based on limits of force (Suchorzewski, et al., 2018; Sinnaie, et al., 2017). In contrast, beam-bond models generally opt for stress- (Brown, et al., 2014; Oñate, et al., 2015) or strain-based failure limits (Carmona, et al., 2008; Schneider, et al., 2010).

Beyond the type of physical property upon which the limit is based, damage models can also be classified by the complexity of their constitutive relationship. In simplistic terms, this means that the damage law can be brittle (Brown, et al., 2014) – a bond disappears upon reaching the failure limit – or ductile – bonds undergo nonlinear hardening or softening upon reaching a critical value. Proponents of nonlinear damage models would argue that such a description is required at the mesoscale to capture the macroscopic ductility displayed by real concrete. Nevertheless, there exist other ways of modelling macroscopic ductility which have shown promising results, i.e. including a stochastic element in the distribution of bond failure limits (Brown, et al., 2014). Moreover, the inclusion of nonlinear stiffness terms may add up to four additional unknown parameters to an already complex mesoscopic model (Sinnaie, 2017; Tran, et al., 2011), greatly convoluting the calibration process and potentially leading to model- or experiment-related over-calibration (Coetzee, 2017).

1.2.3 DEM Mesoscopic properties of concrete

A great portion of DEM concrete studies to date have focused on, and been successful in developing new contact models and formulations that are able to adequately capture concrete behaviour at the bulk level (Nitka & Tejchman, 2015;
Brown, et al., 2014). In spite of these advances, relatively fewer studies have used the advanced capabilities of DEM to critically interrogate the observed mesoscopic phenomena, and more crucially, use the resulting insights to infer what the fundamental mesoscopic properties of concrete are and how these are best represented by various geometrical and mechanical DEM parameters.

### 1.2.3.1 Geometrical properties

Geometrical properties, those which describe a DEM specimen’s initial particle packing, have been shown to significantly affect numerical outcomes depending on the parameter of interest and should be carefully considered when generating the initial packing structure (Chung & Ooi, 2007). Traditionally, the geometrical properties of DEM packings are described qualitatively by concepts such as homogeneity and isotropy and quantitatively by a set of standard packing parameters including porosity, fineness (i.e. number of particles), particle size distribution and dispersion.

#### A. Porosity

Pertaining to the first of these parameters; within the context of concrete-specific DEM studies, the literature reports porosities ranging from 25% (Suchorzewski, et al., 2018) to 46% (Tran, et al., 2011). The significant variation in packing porosities used is in part due to differences between single-phase and multi-phase methods and suggests that packing porosity is likely not a critical parameter. In addition, there is currently no consensus on what constitutes an optimal packing porosity, if such a concept exists at all. Sinnaie (2017) uses ‘high compacity’ (minimal porosity) as one of two primary criteria to determine whether a packing is suitable, however, no quantifiable criterion is provided. Alternatively, in studying the behaviour of linear elastic materials (not concrete), André et al. (2012) concluded that packing porosities should be lower than 36% as this critical value ensures geometrical isotropy for any 3D spherical particle packing. Lastly, concerning the quantifiable influence of packing porosity on specimen bulk behaviour, Nitka & Tejchman (2015) discovered that reducing packing porosity resulted in greater initial stiffness and strength as well as lower ductility. Similarly, Ren et al. (2015) determined that there exists an inversely proportionate relationship between a
concrete specimen’s predicted strength and its void volume fraction (porosity), however, this study considered the tensile strength of concrete only.

B. Heterogeneity

In their study on cementitious rock-type materials, Rojek et al. (2012) found that highly heterogeneous specimens – characterised by higher packing porosities; a greater range of particle sizes; and less evenly dispersed particle size distributions – display more rapid damage development, greater spatial distribution of damage and increased ductility. In addition, the study concluded that as heterogeneity increases, packings become significantly more sensitive to local mechanical parameters. Sinnaie (2017) proposes that the latter conclusion is a testament to adopting a multi-phase approach to modelling concrete, implying that concrete itself is ‘too heterogeneous’ to be represented by a global set of interaction parameters. Since many recent concrete-specific DEM studies have adopted a multi-phase approach (Skarżyński, et al., 2015; Murali & Deb, 2018), packing heterogeneity has not been considered an input parameter in these cases as the aggregate and mortar particle sizes and positions are taken directly from experimental data.

C. Particle size

The influence of packing fineness, or particle size, presents arguably one of the most complicated problems with regard to geometrical packing parameters as it directly relates to the size effect problem observed in real concrete (Bažant, 2000). On the topic of particle size, the literature reports varying results. Nitka & Tejchman (2015) found that a reduction in minimum particle size had no effect on compressive strength but led to an increased pre-peak loss of stiffness and post-peak ductility. On the other hand, Sinnaie (2017) discovered that, while keeping all else constant, an increase in specimen size, which, assuming no change in particle size distribution per unit volume, can be equated to a reduction in mean particle size, led to a decrease in compressive strength and a steeper, more brittle post-peak softening response in line with experimental observations by van Mier, et al. (1997). Lastly, Murali & Deb (2018) noted that the influence of specific DEM parameters changes with specimen size, leading to a size effect reversal in the case of large specimens. This change was attributed to the increase in confining pressure in the interior of large specimens.
1.2.3.2 Mechanical properties

Unlike geometrical properties, mesoscopic mechanical properties are difficult to determine from experimental measurements (Nguyen, et al., 2017). As such, mechanical parameters used in DEM models are mostly determined based on an iterative approach whereby parameters are adjusted until numerical results agree with predicted bulk responses (Coetzee, 2017). One of the shortcomings of this approach is that the resulting chosen mechanical parameters are often not carefully analysed with respect to the physical phenomena they represent and that each contact model and experiment is accompanied by a different set of calibrated mechanical parameters, e.g. the study by Nguyen, et al. (2017). In other words, improper use of the method may lead to calibration of the contact model or experiment rather than the material.

A. Force-displacement parameters

Two of the most fundamental mechanical parameters common to all DEM constitutive models are contact (or bond) normal stiffness and shear stiffness. These parameters may be defined explicitly, as is often the case with contact-bond models (Sinnaie, 2017) or implicitly, i.e. from other parameters such as particle Young's modulus (Nitka & Tejchman, 2015) or bond Young's modulus (Brown, et al., 2014). In terms of selecting and calibrating these stiffness parameters, most studies report a linear relationship between contact normal stiffness and macroscopic Young's modulus (Brown, et al., 2014; André, et al., 2012). Nonetheless, the specific value of the coefficient describing the relationship varies significantly between studies, suggesting that the latter is highly sensitive to the contact model used. In contrast, the influence of the normal-to-shear stiffness ratio has not been extensively studied. Although prior studies report to have used values for this ratio anywhere between 2.5 (Sinnaie, et al., 2017) and 5 (Nitka & Tejchman, 2015), it is uncertain whether the values used in different studies can be directly compared with each other given that different contact models were used in each case. Seeing as this ratio has been shown to impact resulting constitutive behaviour (Brown, 2013), there is a need to determine whether this effect is significant enough to be considered more seriously in future studies.
1.2 Literature review

B. Failure parameters

In similar fashion to the force-displacement parameters, a wide range of bond failure limit values has been used in previous works. Considering only stress- and force-based criteria, the tensile-to-shear strength ratios reported in the literature fall in the range of 0.18 (Nitka & Tejchman, 2015) to 22.3 (Murali & Deb, 2018) and are often selected based on qualitative reasons such as assuming that the mesoscopic tensile-to-shear strength relationship is similar to the macroscopic one (Brown, 2013). Moreover, it has been shown that this ratio can significantly alter the dominant mesoscopic failure mode and that each of these failure modes (tensile and shear) in turn produces noticeably different stress-strain behaviours and fracture patterns (Rojek, et al., 2012). One such example is that shear-dominant meso-failure has been observed to lead to horizontal macro-cracking (Brown, 2013), an occurrence which is traditionally not observed in experimental tests. Nevertheless, few studies report behavioural characteristics beyond macroscopic stress-strain curves and limited emphasis is placed on ensuring that models capture the correct qualitative behaviour (failure plane, Poisson effect) in addition to being able to quantitatively predict bulk properties such as strength and stiffness.

Although past attempts have been made to analyse DEM results at a more profound level, e.g. by presenting inter-particle force chains, particle rotations, displacement fluctuations, local porosity changes and local energies (Skarżyński, et al., 2015; Suchorzewski, et al., 2018), these figures are often no more than alternative ways of visualising results and have yet not resulted in any actionable recommendations. Seeing as concrete behaviour can be described in many more ways than merely by the forces and displacements measured at the loading plates, there is an opportunity to use numerical methods such as the DEM to explore ways to study concrete beyond the superficial boundary data. The resulting insights can subsequently be used to advance knowledge of concrete behaviour at a fundamental level.

1.2.4 Summary

The literature review reveals that many different approaches have been taken to the modelling of concrete using a DEM approach. The key issue identified is that,
although studies have been able to show varying degrees of qualitative and quantitative agreement between DEM results and bulk experimental observations, the question as to what mesoscopic phenomena fundamentally cause these macroscopic behavioural changes remains unanswered in many situations. As such, there is an opportunity to make use of the plethora of discrete data inherently provided by the DEM to critically interrogate the obtained results and to subsequently find the principal relationships between the macroscopic and mesoscopic properties of concrete.

1.3 Aims and Objectives

This thesis aims to advance the understanding of DEM modelling of concrete and work towards developing a scalable, mesoscopic representation of concrete, applicable to a wide range of engineering situations.

To achieve this aim, an existing verified bonded contact model capable of replicating the behaviour of concrete (Edinburgh Bonded Particle Model) will be adopted to conduct a series of comprehensive parametric investigations in order to critically assess the significance of various mesoscopic parameters and their contribution to concrete’s response to load.

Secondary aims are to identify optimal ways in which to analyse and interpret the abundance of DEM data to infer what the macroscopic and mesoscopic properties of concrete are under various conditions. To this point, knowledge and techniques from the fields of discrete element modelling and concrete structural analysis will be combined.

1.4 Structure of thesis

This thesis is presented in five chapters; a brief summary of the contents of each is given below:

Chapter 2 describes the computational methodology adopted in this thesis. The theory behind the contact model of interest, the EBPM, is described, as are the various model parameters and numerical procedures relevant to the discussions in later chapters.
Chapter 3 presents the first part of the parametric investigation focusing on the influence of initial bond fabric parameters. A full set of results concerning the model’s geometrical input parameters obtained by means of a collective research effort are analysed to establish confidence that the discrete bond fabric chosen to depict the concrete specimen is represented in an optimal way. Moreover, the critical bond fabric parameters are identified and relationships between these and the resulting bulk behaviour are derived and expressed quantitatively.

Chapter 4 presents the second part of the parametric investigation which focuses on the influence of the model’s mechanical parameters. New approaches to analyse and interpret DEM simulation data are presented to determine the influence of mesoscopic strength and stiffness parameters on bulk properties such as compressive strength and macro-crack patterns. In addition, a relationship between mesoscopic failure criteria and bulk compressive strength is developed and the procedure is generalised to be applicable in future studies.

Chapter 5 summarises the general conclusions that can be drawn from this thesis and provides recommendations for future work.
Chapter 2  Methodology

2.1 Introduction

This chapter presents the methodology used to obtain the results upon which the discussions in Chapters 3 and 4 are built. It first presents a review of the Discrete Element Method and then provides a comprehensive overview of the contact model adopted in this work, the Edinburgh Bonded Particle model (EBPM). Finally, the main operating procedures for the numerical implementation of the uniaxial compression tests used for parametric studies are presented from beginning to end.

One of the aims of this study is to critically assess the significance of mesoscopic parameters and their contribution to concrete’s response to load. Due to the variety of methods and contact models used by researchers in the field, it is often not possible to directly compare the critical mesoscopic parameters identified in each separate study. As such, it is worth noting that the specific nature in which these parameters appear in every model, including in the EBPM, is only of limited interest. More importantly, however, is questioning the underlying mechanical phenomena caused by these parameters and how these may fundamentally affect the eventual observable macroscopic response.

2.2 The Discrete Element Method

The Discrete Element Method computes the dynamic interaction of elements through an explicit numerical time-stepping scheme whereby a three-stage calculation cycle is carried out during each time step. The cycle is shown in the process flowchart in Figure 2.1.
2.3 The Edinburgh Bonded Particle Model

The Edinburgh Bonded Particle Model (EBPM) is a bonded particle model developed by Brown, et al. (2014) to study the behaviour of cementitious materials. The model is based on the assumption that cementitious materials may be idealised as a compact assembly of spherical, rigid particles connected by bonds.

2.3.1 Contact model parameters

Particles in the EBPM interact at either bonded or non-bonded contacts, which are modelled by the Timoshenko Beam Bonded-Contact Model (TBBM) and the Hertz-Mindlin Contact Model (HMCM) respectively. A comprehensive description of the development of both components of the EBPM is available in Nick Brown’s doctoral thesis (2013). The parameters and equations of interest, those which govern the mesoscopic force-displacement relationships, are presented here.
2.3 The Edinburgh Bonded Particle Model

2.3.1 Bonded contact parameters

A. Bond elastic parameters

Bonded contacts represent cementitious effects by considering discrete particles to be connected by massless virtual bonds whose structural behaviour is described by Timoshenko beam theory (Timoshenko, 1922). These bonds connect rigidly to the centres of two bonded particles and therefore each end of the bond shares the same six degrees of freedom with the particle.

Consider two particles A and B as shown in Figure 2.2. Bond formation occurs when their respective contact radii overlap. The contact radius $r_C$ is defined as:

$$ r_C = \eta \cdot r_p $$

(2.1)

where $\eta$ is the contact radius multiplier and $r_p$ the particle’s physical radius.

Figure 2.2 Example showing an overlap in the contact radii of particles A and B.

Adapted from Brown (2013).

Note that although particles A and B are not in physical contact, they can still be bonded as the contact radius of a particle will generally be set to a value greater than its physical radius.

Following bond formation, the geometric properties of the bond are determined by the positions and sizes of the particles it connects. Again, consider the same two particles A and B, this time connected by a cylindrical beam (bond) as
displayed in Figure 2.3. Bond length $L_b$ and bond radius $r_b$ are calculated by Equations (2.2) and (2.3) respectively.

$$L_b = \|P_B - P_A\|$$  
(2.2)

$$r_b = \lambda \cdot \min(r_A, r_B)$$  
(2.3)

where $P_A$ and $P_B$ are the spatial coordinates of the particles’ respective centres and $r_A$ and $r_B$ are the particle radii. The parameter $\lambda$ is the bond radius multiplier which has a default value of one but may be adjusted according to the user’s needs.

As mentioned earlier, Timoshenko beam theory, suited for stocky beams where shear deformation is important, is used to relate each bond’s internal forces and moments to the particle displacements and rotations. In each time step, the incremental forces are computed from the incremental displacements:

$$\{\Delta F\} = [K] \cdot \{\Delta U\}$$  
(2.4)

where $\{\Delta F\}$ and $\{\Delta U\}$ are the incremental force and displacement vectors respectively and are given by:
\( \{\Delta F\} = \{\Delta F_{\alpha x} \Delta F_{\alpha y} \Delta F_{\alpha z} \Delta M_{\alpha x} \Delta M_{\alpha y} \Delta M_{\alpha z} \Delta F_{\beta x} \Delta F_{\beta y} \Delta F_{\beta z} \Delta M_{\beta x} \Delta M_{\beta y} \Delta M_{\beta z}\}^T \) \hspace{1cm} (2.5)

\( \{\Delta U\} = \{\Delta d_{\alpha x} \Delta d_{\alpha y} \Delta d_{\alpha z} \Delta \theta_{\alpha x} \Delta \theta_{\alpha y} \Delta \theta_{\alpha z} \Delta d_{\beta x} \Delta d_{\beta y} \Delta d_{\beta z} \Delta \theta_{\beta x} \Delta \theta_{\beta y} \Delta \theta_{\beta z}\}^T \) \hspace{1cm} (2.6)

The locations and sign convention of the components of \( \{\Delta F\} \) and \( \{\Delta U\} \) are shown in Figure 2.4. The first subscript denotes the bond end and the second subscript denotes the direction in local coordinates.

![Diagram of forces and moments acting on a bond in the local coordinate system.](image)

Figure 2.4 Forces and moments acting on a bond in the local coordinate system. Taken from Brown, et al. (2015).

Lastly, the local stiffness matrix \([K]\), as presented by Przemieniecki (1986):

\[
[K] = \begin{bmatrix}
    k_1 & \cdots & -k_1 & \cdots & \cdots \\
    -k_1 & k_2 & \cdots & \cdots & \cdots \\
    \cdots & \cdots & k_2 & \cdots & \cdots \\
    \cdots & \cdots & \cdots & k_3 & \cdots \\
    \cdots & \cdots & \cdots & \cdots & k_4 \\
    \cdots & \cdots & \cdots & \cdots & \cdots \\
    \cdots & \cdots & \cdots & \cdots & \cdots \\
    \cdots & \cdots & \cdots & \cdots & \cdots \\
    \cdots & \cdots & \cdots & \cdots & \cdots \\
    \cdots & \cdots & \cdots & \cdots & \cdots \\
\end{bmatrix}
\] \hspace{1cm} (2.7)
Here, $k_1$ constitutes the axial force component, $k_2$ the shear force component, $k_4$ the torsional component, $k_5$ the bending moment component and $k_3$ and $k_6$ the components which describe the interaction between shear and bending effects (tangential displacements and rotations). The equations are given as:

$$k_1 = \frac{E_b A_b}{L_b} \quad (2.8)$$

$$k_2 = \frac{12E_b I_b}{L_b^3(1 + \phi)} \quad (2.9)$$

$$k_3 = \frac{6E_b I_b}{L_b^2(1 + \phi)} \quad (2.10)$$

$$k_4 = \frac{E_b I_b}{L_b(1 + \nu_b)} \quad (2.11)$$

$$k_5 = \frac{E_b I_b (4 + \phi)}{L_b(1 + \phi)} \quad (2.12)$$

$$k_6 = \frac{E_b I_b (2 - \phi)}{L_b(1 + \phi)} \quad (2.13)$$

where $E_b$ is the bond’s Young’s modulus and $\nu_b$ its Poisson’s ratio. The bond’s cross-sectional area $A_b$ and second moment of area $I_b$ are given by Equations (2.14) and (2.15) respectively. Lastly, the Timoshenko shear coefficient $\phi$ for a circular cross-section is given by Equation (2.16).

$$A_b = \pi r_b^2 \quad (2.14)$$

$$I_b = \frac{\pi r_b^4}{4} \quad (2.15)$$

$$\phi = \frac{20r_b^2 (1 + \nu_b)}{3L_b^2} \quad (2.16)$$

To summarise, the mesoscopic parameters which govern the elastic behaviour of the EBPM are:
2.3 The Edinburgh Bonded Particle Model

- **Contact radius multiplier** $\eta$: For a given particle assembly, this parameter influences the total number of bonds generated and as a consequence directly affects fabric stiffness and load resistance.

- **Bond radius multiplier** $\lambda$: As bond radii are a function of $\lambda$, this parameter influences each of the bond stiffness components and hence the stiffness of the overall bond fabric.

- **Particle radius** $r$: Particle radius is the other variable in the bond radius calculation and as such directly influences the values of each of the bond stiffness components and the stiffness of the overall bond fabric. Note that because this formulation of the Timoshenko bond is scale-invariant (Obermayr, et al., 2012), a bond’s individual stiffness will scale proportionally with particle radius.

- **Bond Young’s modulus** $E_b$: As is clear from Equations (2.8) to (2.13), this parameter directly influences each of the local stiffness components and hence the stiffness of the overall bond fabric.

- **Bond Poisson’s ratio** $\nu_b$: Similar to $E_b$, this parameter affects the local stiffness calculation. In particular, this parameter represents the axial-shear stiffness ratio. An increase in $\nu_b$ leads to lower relative shear resistance of the bond.

**B. Bond failure parameters**

The EBPM assumes bonds to behave in a linear elastic and brittle manner. Three independent strength limits are considered: compressive $\sigma_C$, tensile $\sigma_T$ and shear $\tau$. A bond will fail (i.e. disappear) if any of the following criteria are met:

\[
\sigma_C < \sigma_{C_{MAX}} \tag{2.17}
\]

\[
\sigma_T < \sigma_{T_{MAX}} \tag{2.18}
\]

\[
\sigma_S < \sigma_{S_{MAX}} \tag{2.19}
\]

where $\sigma_{C_{MAX}}$, $\sigma_{T_{MAX}}$ and $\sigma_{S_{MAX}}$ at each time step in each bond are determined from the total internal bond forces (and moments) which are calculated by summing up all incremental forces from the start of the simulation:
\{F\} = \sum \Delta F \quad (2.20)

In addition, the stress limits are given by:

\[ \sigma_C = S_C((\zeta_C N) + 1) \quad (2.21) \]
\[ \sigma_T = S_T((\zeta_T N) + 1) \quad (2.22) \]
\[ \sigma_S = S_S((\zeta_S N) + 1) \quad (2.23) \]

where \( S_C \), \( S_T \) and \( S_S \) are user-specified mean bond strengths; \( \zeta_C \), \( \zeta_T \) and \( \zeta_S \) are user-specified coefficients of variation and \( N \) a random number drawn from a normal distribution with a mean of zero and a standard deviation of one. As such, the value of each bond’s strength is allowed to vary between zero and two times the mean bond strength.

Summing up, the mesoscopic parameters which govern the failure criteria of the EBPM are:

- **Mean compressive strength** \( S_C \): This parameter directly influences a bond’s ability to withstand compressive stresses.
- **Mean tensile strength** \( S_T \): This parameter directly influences a bond’s ability to endure tensile stresses.
- **Mean shear strength** \( S_S \): This parameter directly influences a bond’s ability to endure shear stresses.
- **Coefficient of variation** \( \zeta \): If utilised, this parameter influences each bond’s likelihood of possessing a bond strength which differs from the mean.

### 2.3.1.2 Non-bonded contact parameters

In the EBPM, non-bonded contacts appear where two particles come into physical contact either through breakage of bonds or from two particles coming into contact for the first time. Additionally, contacts between particles and external geometries are also considered to be non-bonded. In these situations, the widely-used Hertz-Mindlin Contact Model is used to describe the frictional force-
displacement relationship. A brief overview of the HMCM is presented here. For a comprehensive summary, the reader is referred to the work of Johnson (1987).

At non-bonded contacts, the normal force \( F_n \) and the tangential force \( F_t \) are computed as the summation of their respective spring forces, \( F_{ns} \) or \( F_{ts} \) and damping forces \( F_{nd} \) or \( F_{td} \):

\[
F_n = F_{ns} + F_{nd} \quad (2.24)
\]
\[
F_t = F_{ts} + F_{td} \quad (2.25)
\]

where

\[
F_{ns} = \frac{4}{3} E^* \sqrt{r^*} \delta_n^{1.5} \quad (2.26)
\]
\[
F_{nd} = -2 \sqrt{\frac{5}{6}} b_d \sqrt{S_n m^* V_{n,\text{relative}}} \quad (2.27)
\]
\[
F_{ts} = -S_t \delta_t \quad (2.28)
\]
\[
F_{td} = -2 \sqrt{\frac{5}{6}} b_d \sqrt{S_t m^* V_{t,\text{relative}}} \quad (2.29)
\]

and where \( E^* \) is the equivalent Young’s modulus of the two particles, \( r^* \) is the equivalent radius, \( \delta_n \) and \( \delta_t \) are the normal and tangential overlap, \( b_d \) is a damping ratio related to the coefficient of restitution, \( m^* \) is the equivalent mass, \( V_{n,\text{relative}} \) is the normal component of the relative velocity and \( V_{t,\text{relative}} \) is the tangential component of the relative velocity. Lastly, the tangential force satisfies the Coulomb friction equation:

\[
F_t - \mu_s F_n \leq 0 \quad (2.30)
\]

When considering the significance of the non-bonded contact parameters it is important to note that the nonlinear Hertz-Mindlin Contact model is scale-invariant (Feng, et al., 2009) in 3D meaning that the interaction law is independent of particle size. Furthermore, previous work by Brown (2013) has suggested that non-bonded
contact parameters are generally less influential on the macroscopic response than bonded contact parameters due to the fact that non-bonded contacts only occur in the latter stage of a simulation. For these reasons, only two non-bonded contact parameters are studied in this work. These are:

- **Particle-particle static friction** $\mu_{pp}$: As tangential force is limited by Coulomb friction; this parameter controls the tangential load bearing capacity of non-bonded contacts between particles.

- **Particle-geometry of static friction** $\mu_{pg}$: This parameter alters the behaviour of particles touching the loading plate by limiting the maximum frictional force between these particles and the external geometry.

To conclude, each of the parameters discussed in this section appears either directly or indirectly in the model’s mesoscopic force-displacement relationship. Whilst the influence of each individual parameter at the mesoscale can be simply derived from the equations presented, their combined influence on bulk behaviour quickly becomes very complicated due to the various relationships and interdependencies between them. In fact, preserving simplicity at the mesoscale in order to better understand the root causes of bulk level mechanical behaviour is one of the reasons for opting for simple yet mechanistically robust contact laws in favour of some of the more complex contact models available.

### 2.3.2 Model verification

A brief model verification procedure is presented here to establish confidence that the computational model is robust and accurately represents the underlying mathematical model. Simple verification tests are conducted for the bonded and non-bonded contact models and results are compared with analytical solutions. All simulations are carried out in commercial discrete element software EDEM®.

#### 2.3.2.1 Verification of the Hertz-Mindlin contact model

Verification of the HMCM contact model is carried out using the simple benchmark test described in Chung & Ooi (2011). The test considers the elastic normal impact of two identical spheres with initial velocities of 10 m/s going in opposite directions. The analytical solutions for maximum contact displacement and
force are given by Equations (2.31) and (2.32) respectively (Timoshenko & Goodier, 1970). Force-displacement curves of the impacts are shown in Figure 2.5.

\[
d_{c,max} = \left[\frac{5\sqrt{2}\pi\rho(1-\nu^2)}{4E}\right]^{\frac{5}{2}}rV_{rela}^{\frac{4}{5}}
\]

(2.31)

\[
F_{max} = \left[\frac{2}{9}\frac{rE^2}{(1-\nu^2)^2}\right]^{\frac{1}{2}}d_{c,max}^{\frac{3}{2}}
\]

(2.32)

where \( E \) is the particle Young’s modulus, \( \rho \) its density, \( r \) its radius, \( \nu \) its Poisson’s ratio, and \( V_{rela} \) the relative velocity of the two spheres.

Figure 2.5 Analytical and numerical force-displacement curves of the elastic normal impact of two identical spheres. Analytical curves taken from Chung & Ooi (2011).

2.3.2.2 Verification of the Timoshenko Beam Bonded-Cn

Next, the EBPM’s bonded contact model, the TBBM is verified by simulating a simply supported circular Timoshenko beam undergoing free vibration. A three-particle model is created with TBBM bonds representing a circular steel beam with section properties \( E = 200 \) GPa; \( \nu = 0.3 \); \( r = 0.1 \) m; \( L = 6 \) m; and carrying a central
mass of \( m_c = 1000 \text{ kg} \). Figure 2.6 shows the transition from the idealised mathematical model to the computational model in EDEM.

![Figure 2.6 Conceptual and computational model of a simply supported beam.](image)

Using Equation (2.33) (Ross, et al., 1999), the theoretical natural frequency of the beam is found to be \( f_n = 9.392 \text{ Hz} \).

\[
f_n = \frac{1}{2\pi} \sqrt{\frac{192E_b l_b G_b A_b}{m_b (4L_b^3 G_b A_b + 48f_s E_b l_b L_b)}}
\]  

(2.33)

By plotting the central displacement-time curve shown in Figure 2.7, the natural frequency of the numerical model was found to be \( f_n = 9.346 \text{ Hz} \). The 0.5% error is speculated to be due to the ‘artificial’ implementation of boundary conditions. Since EDEM does not offer the option to explicitly introduce displacement boundary conditions, the translational restrictions at either end of the beam were imposed by encapsulating the particles with square geometries. This manner of fixing the particles likely led to a slightly more flexible overall system, displayed by a lower fundamental frequency.
2.4 Numerical implementation

This section lays out the operational procedures involved in setting up a robust numerical simulation which accurately embodies the displacement-controlled uniaxial compression test. These include: particle generation using the rearrangement algorithm R-Ball, running DEM simulations in EDEM and finally post-processing results in EDEM and in third-party software P4 (Particle-Analytics).

2.4.1 Particle generation

In similar fashion to the original work by Brown (2013), this study makes use of the collective particle rearrangement technique, R-Ball (Labra & Oñate, 2009) to obtain the desired high-density packings. The rearrangement technique involves first creating a ‘prototype’ particle packing of a user-specified porosity by allowing particle overlaps to exist, and by subsequently rearranging and removing particles through an iterative optimisation algorithm whereby particles with overlaps greater than a set limit are removed from the packing. The porosity \( n \) of a particle packing is defined as follows:

\[
T_P = 0.107 \Rightarrow f_P = 9.346 \text{ Hz}
\]

\[
\text{Error} \approx 0.5\%
\]

Figure 2.7 Displacement-time plot used to determine the fundamental frequency.

Additional successful verification tests carried out by Brown (2013) include a static beam bending test as well as individual tests on the pure tensile, torsional, and bending response of a single bond.
2.4 Numerical implementation

\[ n = 1 - \frac{V_S}{V_T} \]  

(2.34)

where \( V_S \) denotes the volume of the particles and \( V_T \) denotes the total volume.

The target particle packing is defined by the user through a set of input parameters which include mean particle radius, particle size distribution (e.g. uniform, normal, log-normal) and a series of numerical parameters such as the maximum number of iterations and overlap limits. Among these numerical parameters, the maximum overlap limit is most influential as it determines the resulting packing porosity and hence indirectly affects bond fabric density. The general step-by-step process used to generate high-density packings is shown in Figure 2.8.

1. **Choose packing parameters**: minimum, mean and maximum particle radii as well as particle size distribution depending on desired packing properties.

2. **Set ‘target’ porosity**: it is recommended to choose an unrealistically low value, i.e. 15% as porosity will increase once algorithm begins removing particles.

3. **Set maximum allowable overlap limit**: depending on this limit, the algorithm will optimise particle positions to reach the densest possible packing. Higher overlap limits correspond to denser packings.

4. **Run algorithm**: let the algorithm run for up to 20,000 global iterations.

5. **Post-process results**: post-process R-Ball results (e.g. using GiD) and import particle position data into existing EDEM simulation deck.

Figure 2.8 Step-by-step procedure to generate high-density packings in R-Ball.
2.4 Numerical implementation

2.4.2 DEM simulation of a uniaxial compression test of a concrete cylinder: Reference case

All simulations in this study mimic a displacement-controlled uniaxial compression test of concrete as described in most structural design codes, including The British Standards (BS EN 12390-3, 2012) and ASTM International (ASTM Standard CCA C09.61, 2012). Following initial model testing and based on recommendations provided by the literature, a reference case specimen was built to represent the concrete cylinder. In addition, a series of numerical implementation parameters and operational procedures were selected to optimally mimic the actual experimental procedure.

2.4.2.1 Reference parameters

A comprehensive list of specimen geometrical and mechanical parameters and their values are provided in Table 2.1. All reference values were chosen either based on recommendations made by Brown (2013) or by comparing parameters to similar ones used in other studies. The highlighted (green) rows indicate the parameters which are investigated in Chapters 3 and 4 and were selected based on the questions identified in the literature review.
2.4 Numerical implementation

Table 2.1 Packing, bonded and non-bonded parameters for the reference case.

<table>
<thead>
<tr>
<th>Type</th>
<th>Parameter</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Packing</td>
<td>$H_0$</td>
<td>Initial specimen height (mm)</td>
<td>200</td>
</tr>
<tr>
<td></td>
<td>$D_0$</td>
<td>Initial specimen diameter (mm)</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>$P$</td>
<td>Total number of particles</td>
<td>28836</td>
</tr>
<tr>
<td></td>
<td>$n$</td>
<td>Porosity</td>
<td>0.33</td>
</tr>
<tr>
<td></td>
<td>$r_{avg}$</td>
<td>Average particle radius (mm)</td>
<td>2.0</td>
</tr>
<tr>
<td></td>
<td>$r_{max}$</td>
<td>Maximum particle radius (mm)</td>
<td>2.8</td>
</tr>
<tr>
<td></td>
<td>$r_{min}$</td>
<td>Minimum particle radius (mm)</td>
<td>1.2</td>
</tr>
<tr>
<td></td>
<td>$\xi$</td>
<td>Radius ratio</td>
<td>2.3</td>
</tr>
<tr>
<td></td>
<td>$\eta$</td>
<td>Contact radius multiplier</td>
<td>1.1</td>
</tr>
<tr>
<td>Non-bonded</td>
<td>$\rho_p$</td>
<td>Particle density (kg m$^{-3}$)</td>
<td>2700</td>
</tr>
<tr>
<td></td>
<td>$E_p$</td>
<td>Particle Young’s modulus (GPa)</td>
<td>30</td>
</tr>
<tr>
<td></td>
<td>$\nu_p$</td>
<td>Particle Poisson’s ratio</td>
<td>0.25</td>
</tr>
<tr>
<td></td>
<td>$\mu_{sp}$</td>
<td>Particle-particle static friction</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td>$\mu_{rp}$</td>
<td>Particle-particle rolling friction</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>$\mu_{sg}$</td>
<td>Particle-geometry static friction</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td>$\mu_{rg}$</td>
<td>Particle-geometry rolling friction</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>$e_p$</td>
<td>Particle-particle restitution</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td>$e_g$</td>
<td>Particle-geometry restitution</td>
<td>0.0001</td>
</tr>
<tr>
<td>Bonded</td>
<td>$E_b$</td>
<td>Bond Young’s modulus (GPa)</td>
<td>50</td>
</tr>
<tr>
<td></td>
<td>$\nu_b$</td>
<td>Bond Poisson’s ratio</td>
<td>0.2</td>
</tr>
<tr>
<td></td>
<td>$\lambda$</td>
<td>Bond radius multiplier</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td>$\sigma_c$</td>
<td>Mean bond compressive strength (MPa)</td>
<td>500</td>
</tr>
<tr>
<td></td>
<td>$\sigma_T$</td>
<td>Mean bond tensile strength (MPa)</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>$\sigma_S$</td>
<td>Mean bond shear strength (MPa)</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>$\zeta_c$</td>
<td>COV* of compressive strength</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>$\zeta_T$</td>
<td>COV* of tensile strength</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td>$\zeta_S$</td>
<td>COV* of shear strength</td>
<td>1.0</td>
</tr>
</tbody>
</table>

*Coefficient of Variation

2.4.2.2 Numerical implementation parameters

With any computational model, there are a number of numerical parameters that need to be carefully considered to ensure the numerical stability of a simulation without compromising its ability to represent reality. In this study, these are the time step $\Delta t$, the loading-strain rate $L_r$ and the global damping coefficient $\zeta_d$. These
2.4 Numerical implementation

numerical parameters have been studied in depth in the literature (Cho, et al., 2007; Brown, 2013) and as such only a brief overview is presented here.

The approach adopted in choosing the time step in this study follows the method by O’Sullivan & Bray (2004) whereby the time step is determined as a fraction (0.1 – 0.2) of the critical time step. The equations used to determine the critical time step for both bonded and non-bonded contacts are presented in Brown, et al. (2014). The two remaining numerical parameters, loading rate $L_r$ and global damping coefficient $\iota_d$, are selected based on the parametric studies conducted by Brown (2013) where it was shown that a loading rate of $1 \varepsilon s^{-1}$ or less should be used and that global damping is not required to achieve numerical stability.

For all the simulations in this thesis, the time step used will be taken as $10^{-7}$ s which is approximately 5% of the critical time step in all cases. The loading rate used is $200 \text{mm s}^{-1}$, or $1 \varepsilon s^{-1}$ given that all specimens have a height of $200 \text{mm}$. Finally, global damping is set to zero. A summary of the numerical implementation parameters used for all simulations is shown in Table 2.2.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta t$</td>
<td>Time step (s)</td>
<td>$10^{-7}$</td>
</tr>
<tr>
<td>$L_r$</td>
<td>Loading rate (mm.s$^{-1}$)</td>
<td>200</td>
</tr>
<tr>
<td>$\iota_d$</td>
<td>Global damping coefficient</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 2.2 Summary of numerical implementation parameters.

2.4.2.3 Numerical smoothing of boundary surfaces

A question that emerged early on in the modelling process was whether or not it was necessary to consider the effects of specimen boundary roughness when performing the numerical simulations. The literature reports that in DEM as well as in laboratory experiments, local porosity differences in the boundary region may lead to biased grain crushing and an underestimation of the stiffness of a material (Marketos & Bolton, 2010).

Whilst numerical ‘smoothing’ of specimen boundaries to avoid these undesirable effects is certainly a viable approach, preliminary simulations showed that by assigning the EBPM contact law to particle-geometry contacts, particle-
geometry forces originating from initial contact overlaps were removed by the contact model (as are inter-particle contact forces). Hence, applying the EBPM contact law to particle-geometry contacts intrinsically removes the need to consider specimen boundary roughness, although this is admittedly done in an artificial manner. Potential issues related to this approach are discussed in Chapter 3.

2.4.3 Processing and visualisation of results

From an engineering design point of view, the principal bulk properties of a concrete sample are its compressive strength and secant modulus of elasticity (Kovler & Roussel, 2011). As such, a first step in understanding the behaviour of a numerical specimen is to evaluate these properties by computing them from raw simulation data.

2.4.3.1 Computing bulk properties

This section describes how bulk stresses and strains are computed from raw simulation data in order to determine those properties. In addition, the process of calculating a specimen’s bulk Poisson’s ratio and global damage are also presented.

A. Stress

Bulk compressive stress \( \sigma \) is calculated by dividing the average force acting on the loading plates by the contact area between specimen and loading plate. After simplification, this yields the following:

\[
\sigma = \frac{2(F_T + F_B)}{\pi D_g^2} \quad (2.35)
\]

where \( F_T \) and \( F_B \) are the total (compressive) forces acting on the top and bottom loading plates and \( D_g \) is the diameter of either loading plate in contact with the specimen.

B. Strain

Continuum mechanics defines engineering strain as the ratio of total deformation to the initial dimension of the material body. For axial strain, this can be expressed as:
2.4 Numerical implementation

\[ \varepsilon = \frac{h_0 - h}{h_0} \]  \hspace{1cm} (2.36)

where \( h_0 \) and \( h \) are the initial and current height of the specimen respectively.

The height of the numerical specimen at any point in time is defined as the sum of the vertical distance between top and bottom geometries and the average contact normal overlaps at both ends of the specimen as given by Equation (2.37).

\[ h = Z_T - Z_B + \delta_{T,avg} + \delta_{B,avg} \]  \hspace{1cm} (2.37)

where \( Z_T \) and \( Z_B \) are the positions of the top and bottom loading plates, \( \delta_{T,avg} \) the average contact overlap between particles and the top loading plate and \( \delta_{B,avg} \) the average contact overlap between particles and the bottom loading plate. This definition of height differs from simply assessing strain from the positions of the loading plates (see Figure 2.9) and was adopted after initial simulations revealed that alternative measures of height produced unrealistic responses due to the model’s numerical approximations as shown in Figure 2.10.
Figure 2.9 Comparison of different ways to compute specimen height. Adapted from Brown (2013).
Figure 2.10 Three representations of identical simulation data showing the importance of selecting the correct height calculation.

C. **Bulk Young’s modulus**

The measure for bulk stiffness used in this work is the secant modulus of elasticity $E_c$, describing the secant value of the bulk stiffness of the specimen. As concrete is only partially elastic, this property should be evaluated when loading is still in the near elastic range, up to roughly 30% to 40% of the ultimate strength (Bamforth, et al., 2007). In this study, the secant elastic modulus is determined using Equation (2.38) when the specimen is subjected to an internal stress equal to 40% of the ultimate strength.

$$E_{c(0.4)} = \frac{\sigma_{(0.4)} - \sigma_{(0)}}{\varepsilon_{(0.4)} - \varepsilon_{(0)}}$$  \hspace{1cm} (2.38)

D. **Bulk Poisson’s ratio**

The Poisson’s ratio $\nu_c$ describes the ratio of the radial $\varepsilon_r$ to axial $\varepsilon$ strain. In similar fashion to the secant elastic modulus, the Poisson's ratio is calculated when loading is at 40% of the ultimate strength, such that:
2.4 Numerical implementation

\[ v_{c(0.4)} = \frac{-\varepsilon_{r(0.4)}}{\varepsilon_{(0.4)}} \]  

(2.39)

where \( \varepsilon_{(0.4)} \) is calculated using Equation (2.36) and radial strain \( \varepsilon_{r(0.4)} \) is computed by tracking the lateral displacements of pairs of particles lying opposite to each other at the specimen’s mid-height as displayed in Figure 2.11.

Figure 2.11 Diagrammatic representation of the determination of specimen width. Adapted from Brown (2013).

The radial strain is determined using Equation (2.40):

\[ \varepsilon_{r} = \frac{D - D_0}{D} \]  

(2.40)

where \( D \) is the width of the specimen and is given by:

\[ D = \text{mean}(d_j), \quad \text{for } j = 1, 2, ... \]  

(2.41)

Clearly, the calculated \( v_c \) gets more accurate as one increases the number of particles tracked. However, tracking individual particles proved to be a moderately
cumbersome procedure and tracking merely two pairs of particles was sufficient to provide adequate estimations for the bulk Poisson’s ratio in all cases.

E. Bond breakage and damage

In the EBPM, crack propagation occurs at the particle scale and is represented by bond failure. Internal damage caused by the breakage of bonds can be tracked at the bulk level by considering the ratio of broken bonds to total initial bonds. In addition, the model keeps track of local damage in a similar manner by calculating damage for each particle in the simulation using Equation (2.42).

\[
D_m = 1 - \frac{B}{B_0}
\]  

(2.42)

where \(D_m\) is local damage, \(B\) is the number of bonds connected to that particle at the current time step and \(B_0\) denotes the initial number of bonds connected to that particle.

2.4.3.2 Visualising damage using EDEM and Particle Analytics (P4)

This thesis makes use of the post-processing capabilities of EDEM and third-party post-processing software P4. Whereas the former provides discrete representations of direct simulation data, the latter offers the ability to translate discrete data into an equivalent continuum format through spatial averaging (Particle Analytics Ltd). Both techniques are used throughout this text, however, P4 is especially useful when demonstrating internal stresses and strains where averaged results are able to provide a much clearer visual representation than discrete results would. Figure 2.12 highlights the difference between the two techniques for the property 'local damage'.
Figure 2.12 Local damage $D_m$ plot represented in (a) discrete format and (b) continuum format using P4.

3.1 Introduction

This chapter presents the first part of a parametric study that investigates the influence of model parameters on the DEM simulation of the uniaxial compression test described in Chapter 2. Here, the focus is on the influence of the bond fabric (geometrical) parameters only.

As revealed in the literature review, the geometry of a discrete concrete specimen can be presented either using a single- or multi-phase approach. Given that one of the primary aims of this study is to use the EBPM to work towards developing a scalable, mesoscopic representation of concrete which can eventually become applicable to a wide range of engineering problems, the approach taken in this study considers concrete as a single-phase material. Here, mesoscale is defined as an intermediate length-scale where both geometrical and mechanical heterogeneities are clearly present, but where grain-level details remain excluded. It should be noted, therefore, that in contrast to other mesoscale DEM concrete studies discussed in Chapter 2 (Skarżyński, et al., 2015; Sinnaie, et al., 2017), the packings presented are not intended to possess a fully microscopic description of concrete and as such neither the particles nor the bonds are directly representative of physical entities such as aggregates, cement mortars or interfacial transition zones.

Concerning terminology, certain terms will be used throughout this chapter when referring to the discrete representation of concrete; the differences are subtle but important. A ‘packing’ refers solely to the assembly of spherical particles that make up the discrete sample and excludes any association with bonded properties. A ‘bond fabric’ arises after the packing is subjected to the initial bonding time step and refers to the entity which comprises both the physical particles and the virtual cementitious bonds. Finally, the terms ‘sample’ or ‘specimen’ are used interchangeably when alluding to the discrete body as it were a physical concrete specimen.
3.2 Effect of randomised bond strengths

The coefficient of variation (COV) $\zeta$ serves two purposes. Firstly, it introduces a stochastic element into the model that is intended to mimic the inherent mechanical heterogeneity present in concrete. No two laboratory specimens behave in exactly the same way and the COV intends to capture this effect numerically by inducing spatial variation of strength into specimens even when they share the same geometry. The second purpose of the COV is to provide the model with a component of ductility intended to replicate the strain-softening effect observed in experimental studies.

Here, the effect of the COV is investigated with the aim of quantifying the degree of statistical scatter it causes to behaviour at the bulk level. Given that a great portion of the remaining Chapters attempts to study the influence of various mesoscopic parameters, it is important to first quantify how much of the change in response is attributable to the stochastic nature of the model itself rather than a change in any of the deterministic parameters. The values for each of the COV parameters $\zeta_i$ are 0, 1 and 1 for the compressive, tensile and shear components respectively. Five identical specimens, barring their spatial distribution of bond strengths, were subject to uniaxial compression and the bulk stress-strain curves are shown in Figure 3.1. All specimens possess the same reference parameters given in Table 2.1 in the previous chapter. Bulk properties evaluated from the DEM computation are summarised in Table 3.1.
3.2 Effect of randomised bond strengths

Figure 3.1 Stress-strain curves for the reference simulation cases and influence of COV.

Table 3.1 Bulk properties computed from the five reference simulations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Mean</th>
<th>Coefficient of variation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$f_{c'}$</td>
<td>Ultimate strength (MPa)</td>
<td>51.54</td>
<td>4.3%</td>
</tr>
<tr>
<td>$\varepsilon_c$</td>
<td>Axial strain at failure</td>
<td>0.001667</td>
<td>6.9%</td>
</tr>
<tr>
<td>$E_{c(0.4)}$</td>
<td>Secant elastic modulus (GPa)</td>
<td>38.10</td>
<td>1.6%</td>
</tr>
</tbody>
</table>

Given that the three specimens possess identical linear elastic properties, they should exhibit very similar behaviour until the initiation of bond breakage. This is confirmed by the results shown in Table 3.1, where it can be seen that initial bulk stiffness varies by 1.6% from the mean value, ultimate compressive strength varies by 4.3% and axial strain at failure by 6.9%. The magnitudes of the coefficients of variation are lower than what Mokhtar, et al. (2013) observed for the variability of experimentally tested concrete, where it was found that the COV for bulk Young’s modulus ranges from 5.4% to 7.0% and that for compressive strength ranges from 9.0% to 11.3%.
3.3 Influence of packing porosity

In analysing post-peak behaviour, the failure planes obtained for three of the five scenarios presented in Figure 3.2 demonstrate clearly that damage is distributed differently in each specimen, suggesting that the bond fabric’s ‘weakest link’ is greatly dependent on the spatial distribution of bond strengths. Moreover, the slight differences in post-peak residual strength can be attributed to the variation in failure planes seeing as the former is largely dependent on the number of frictional contacts mobilised which depends on the inclination of the macro-crack (Brown, 2013).

![Damage plots at 0.3% strain for simulations (a) A, (b) B and (c) C.](image)

Figures 3.2 Damage plots at 0.3% strain for simulations (a) A, (b) B and (c) C.

Whilst the model's ability to predict variation in peak and post-peak response is desirable in terms of replicating real variability observed in concrete, it adds unwanted noise to the parametric investigation. Although removing the effect of COV is impossible for the remaining parameters in Chapter 3 for obvious reasons, the parametric study in Chapter 4 will consider ways to remove the stochastic effect of the COV without forgoing the necessary ductility it provides by artificially ensuring bond strengths are distributed equally.

3.3 Influence of packing porosity

In order to investigate the influence of packing porosity, four specimens were generated with gradually increasing maximum allowable overlaps (1%-15%) to
obtain progressively denser packings. The resulting packings with porosities ranging from 31.5% to 37.9% were subjected to uniaxial compression and the bulk stress-strain curves are shown in Figure 3.3. In addition, a table summarising the DEM computed bulk properties is presented in Table 3.2.

The results indicate that increasing packing density (reducing porosity) significantly increases bulk ultimate strength and bulk stiffness, matching previous findings where it has been stated that there exists an inversely proportionate relation between predicted strength and porosity (Ren, et al., 2015). The increase in bulk strength and stiffness can be attributed to the greater number of bonds per

---

**Figure 3.3 Influence of packing porosity on the stress-strain response.**

**Table 3.2 Summary of influence of packing porosity on DEM bulk response.**

<table>
<thead>
<tr>
<th>Porosity</th>
<th># Particles</th>
<th>Coordination number</th>
<th>Ultimate strength (MPa)</th>
<th>Strain at ultimate strength</th>
<th>Secant elastic modulus (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>n</td>
<td>P</td>
<td>C</td>
<td>$f_c$</td>
<td>$\varepsilon_c$</td>
<td>$E_{c(0.4)}$</td>
</tr>
<tr>
<td>37.9%</td>
<td>27187</td>
<td>8.27</td>
<td>40.6</td>
<td>0.170%</td>
<td>31.4</td>
</tr>
<tr>
<td>36.0%</td>
<td>27924</td>
<td>8.55</td>
<td>46.0</td>
<td>0.170%</td>
<td>34.4</td>
</tr>
<tr>
<td>33.7%</td>
<td>28836</td>
<td>8.88</td>
<td>51.5</td>
<td>0.166%</td>
<td>38.1</td>
</tr>
<tr>
<td>31.5%</td>
<td>29690</td>
<td>9.19</td>
<td>59.2</td>
<td>0.182%</td>
<td>41.5</td>
</tr>
</tbody>
</table>
3.3 Influence of packing porosity

particle, as displayed by the coordination number shown in Table 3.2. Interestingly, packing porosity does not seem to affect strain at peak stress to the same extent. By the same token, Figure 3.4 shows that the progression of bond breakage is nearly identical for all packings, meaning that the fraction of broken bonds at any loading stage is almost constant across the four simulations. Hence, whilst a denser particle packing results in the presence of more load-carrying bonds (i.e. stiffer) and a greater number of bonds which need to be broken to cause failure (i.e. stronger), the relative rate of bond breakage in response to loading does not change with changing porosity and as a result bulk axial strain at peak strength remains similar for the four cases.

![Figure 3.4 Influence of packing porosity on progression of bond breakage.](image)

Finally, the normalised stress-strain curves displayed in Figure 3.5 next to Lim & Ozbakkaloglu's (2014) empirical stress-strain model for a specimen of the same geometry reveals that varying packing porosity within the range studied has little to no influence on the relative loss of stiffness and post-peak softening slope. This suggests that although packing porosity affects the absolute values of bulk strength and stiffness, it is not a critical parameter in terms of providing a qualitative representation of bulk behaviour. In short, whilst a range of packing porosities can
be used, the influence it has on absolute strength and stiffness means it is important that this parameter is kept constant throughout any subsequent calibration or scaling procedure.

3.4 Influence of particle size distribution

One approach for introducing mesoscopic inhomogeneity caused by air voids and randomly shaped aggregates into a numerical model is to use a polydisperse particle distribution. In addition, the inclusion of particle size disparity in packings can aid in avoiding undesirable directional effects caused by geometrical anisotropy (André, et al., 2012). Here, the influence of increased packing heterogeneity as a result of different particle size distributions is investigated in two ways: first by modifying the nature of the distribution of particle radii (from normal to uniform) and secondly by varying the radius ratio $\xi$ (Equation (3.1)) while keeping mean particle radius constant.

![Graph showing the influence of particle size distribution](image-url)

Figure 3.5 Normalised version of Figure 3.3. Experimental curve by Lim & Ozbakkaloglu (2014).

3.4 Influence of particle size distribution
3.4 Influence of particle size distribution

\[ \xi = \frac{r_{\text{max}}}{r_{\text{min}}} \]  

(3.1)

For each of the packings analysed in the previous section, equivalent packings were generated where the particle sizes were determined following a uniform distribution rather than a normal distribution (as was the case previously) with the intention of increasing overall packing heterogeneity. In addition, mean particle radius and porosity were kept as close to constant as possible. The influence of particle size distribution on resulting DEM bulk properties is summarised in Table 3.3. In addition, Figure 3.6 shows a comparison of the distribution of particle diameters for the two \( n = 34\% \) cases and Figure 3.7 displays stress-strain curves for the \( n = 38\% \) and \( n = 31\% \) simulations.

Table 3.3 Influence of changing between normal and uniform particle size distributions.

<table>
<thead>
<tr>
<th>Distribution type</th>
<th>Porosity</th>
<th>Ultimate strength (MPa) ( f'_c )</th>
<th>Strain at ultimate strength ( \varepsilon'_c )</th>
<th>Secant elastic modulus (GPa) ( E_c(0.4) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Uniform</td>
<td>38%</td>
<td>39.5</td>
<td>0.165%</td>
<td>30.7</td>
</tr>
<tr>
<td>Normal</td>
<td>38%</td>
<td>40.6</td>
<td>0.170%</td>
<td>31.4</td>
</tr>
<tr>
<td>Uniform</td>
<td>36%</td>
<td>44.3</td>
<td>0.177%</td>
<td>33.9</td>
</tr>
<tr>
<td>Normal</td>
<td>36%</td>
<td>46.0</td>
<td>0.170%</td>
<td>34.4</td>
</tr>
<tr>
<td>Uniform</td>
<td>34%</td>
<td>50.1</td>
<td>0.178%</td>
<td>37.5</td>
</tr>
<tr>
<td>Normal</td>
<td>34%</td>
<td>51.5</td>
<td>0.166%</td>
<td>38.1</td>
</tr>
<tr>
<td>Uniform</td>
<td>31%</td>
<td>56.7</td>
<td>0.179%</td>
<td>41.9</td>
</tr>
<tr>
<td>Normal</td>
<td>31%</td>
<td>59.2</td>
<td>0.182%</td>
<td>41.5</td>
</tr>
</tbody>
</table>
3.4 Influence of particle size distribution

Figure 3.6 Comparison of particles sizes between packings generated according to a (a) normal distribution and (b) uniform distribution.
3.4 Influence of particle size distribution

Figure 3.7 Influence of particle size distribution on stress-strain behaviour.

Results indicate that packings with similar porosities exhibit comparable bulk properties, regardless of particle size distribution. Moreover, the difference in relative bond progression between normal and uniformly distributed specimens is minimal as shown in Figure 3.8 and comparable inclined macro-cracks were observed in all specimens suggesting that particle size distribution has no effect on failure plane inclination. In short, for the range of porosities and size distributions investigated, the type of size distribution is relatively unimportant.
3.4 Influence of particle size distribution

In addition to distribution type, packing dispersion, measured by radius ratio $\xi$ (Equation (3.1)) was also studied. Packings with radius ratios ranging from 1.7 to 7 with similar porosities (33-34%) and mean particle radii (2 mm) were tested. Packing properties as a result of changing maximum and minimum particle radii are shown in Table 3.4, stress-strain profiles are displayed in Figure 3.9 and the corresponding DEM computed bulk properties are tabulated in Table 3.5.

Table 3.4 Summary of packing properties due to changes in radius ratio.

<table>
<thead>
<tr>
<th>Radius ratio $\xi$</th>
<th>Minimum particle radius ($r_{\text{min}}$) (mm)</th>
<th>Maximum particle radius ($r_{\text{max}}$) (mm)</th>
<th>Number of particles $P$</th>
<th>Number of bonds $B$</th>
<th>Coordination number $C$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.7</td>
<td>1.5</td>
<td>2.5</td>
<td>29854</td>
<td>134333</td>
<td>9.00</td>
</tr>
<tr>
<td>2.3</td>
<td>1.2</td>
<td>2.8</td>
<td>28836</td>
<td>127994</td>
<td>8.88</td>
</tr>
<tr>
<td>3.0</td>
<td>1</td>
<td>3</td>
<td>27596</td>
<td>120835</td>
<td>8.76</td>
</tr>
<tr>
<td>7.0</td>
<td>0.5</td>
<td>3.5</td>
<td>23569</td>
<td>98056</td>
<td>8.32</td>
</tr>
</tbody>
</table>
3.4 Influence of particle size distribution

Figure 3.9 Influence of radius ratio on stress-strain behaviour.

Table 3.5 Summary of influence of radius ratio on computed bulk properties.

<table>
<thead>
<tr>
<th>Radius ratio ξ</th>
<th>Coordination number C</th>
<th>Ultimate strength $f_c$ (MPa)</th>
<th>Strain at ultimate strength $\varepsilon_c$</th>
<th>Secant elastic modulus $E_{c(0.4)}$ (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.7</td>
<td>9.00</td>
<td>53.7</td>
<td>0.170%</td>
<td>39.2</td>
</tr>
<tr>
<td>2.3</td>
<td>8.88</td>
<td>51.5</td>
<td>0.166%</td>
<td>38.1</td>
</tr>
<tr>
<td>3.0</td>
<td>8.76</td>
<td>48.8</td>
<td>0.170%</td>
<td>36.3</td>
</tr>
<tr>
<td>7.0</td>
<td>8.32</td>
<td>47.3</td>
<td>0.185%</td>
<td>34.3</td>
</tr>
</tbody>
</table>

There is again an apparent trend between increasing a bond fabric’s coordination number, in this case as a consequence of reducing average particle size disparity, and the increase of its bulk strength and stiffness. Furthermore, the normalised curves displayed in Figure 3.10 show that an increase in radius ratio is accompanied by a slightly more ductile pre-peak behaviour, although still not to the same extent as shown by the empirical curve. This increase in ductility can be related to the fact that as packing dispersion increases, a greater range of bond cross-sectional areas is introduced into the fabric resulting in an increasingly heterogeneous distribution of bond stiffnesses. As a consequence, internal damage
3.4 Influence of particle size distribution

progresses at a higher pace and is more spread out in the highly disperse specimens, as can be seen in the damage progression curves in Figure 3.11 and in the cross-sectional damage plots in Figure 3.12. In fact, global damage at ultimate strength is 28% greater when $\xi = 7.0$ than when $\xi = 1.7$. A similar relationship between fabric heterogeneity and ductility was observed in a study on the effect of meso-structure on the tensile strength of concrete where it was concluded that: “this [higher mesoscopic heterogeneity] leads to greater stress distribution, greater dispersion of the available stored energy in the formation of more scattered micro-cracks ... These features retard macro-crack growth, increase macro fracture energy, and allow the specimen to carry higher stresses prior to failure.” (Murali & Deb, 2018).

Figure 3.10 Normalised version of Figure 3.9 highlighting relative loss of stiffness.
Experimental curve by Lim & Ozbakkaloglu (2014).
3.4 Influence of particle size distribution

Figure 3.11 Influence of radius ratio on bond breakage.

Figure 3.12 Damage plots of YZ cross-section at 0.3% strain for (a) $\xi = 1.7$, (b) $\xi = 3.0$ and (c) $\xi = 7.0$ showing influence of radius ratio on damage spread.
3.5 Influence of mean particle size and particle number

To apply the bonded particle model to any geometry, a relationship must be established between the number of particles in a given specimen volume and the resulting bulk behavioural properties. As explained in Chapter 2, both individual components of the EBPM, the TBBM and HMCM, are scale-invariant from a mechanics viewpoint. However, whether this indeed leads to scale-invariance at the bulk level is questionable given the constantly changing dynamics between the two components as damage develops. Moreover, scale-invariance is not necessarily desirable given that real concrete specimens exhibit significant size effects (Bažant, 2000; Sinnaie, 2017).

In this section, the influence of the number of particles is investigated for specimens with between 8.3K and 68.6K particles. Although the coarsest of these packings is arguably too coarse given that previous studies suggest that the minimum number of particles in a 3D volume should be approximately 10K particles (André, et al., 2012), the results are still included. In addition, the scaling procedure led to slight variations between packing porosities as is shown in the summary in Table 3.6. The influence of particle number on stress-strain behaviour is displayed in Figure 3.13, with matching bulk properties provided in Table 3.7.

Table 3.6 Summary of packing properties as a result of changing mean particle size.

<table>
<thead>
<tr>
<th>Mean particle radius (mm)</th>
<th>$r_{avg}$</th>
<th>Radius ratio</th>
<th>Porosity</th>
<th>Number of particles</th>
<th>Number of bonds</th>
<th>Coordination number</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{avg}$</td>
<td>1.5</td>
<td>2.3</td>
<td>33.3%</td>
<td>68,566</td>
<td>308,933</td>
<td>9.01</td>
</tr>
<tr>
<td>2.0</td>
<td>2.3</td>
<td>33.7%</td>
<td>28,836</td>
<td>127,994</td>
<td>8.88</td>
<td></td>
</tr>
<tr>
<td>2.5</td>
<td>2.3</td>
<td>34.2%</td>
<td>14,654</td>
<td>64,055</td>
<td>8.74</td>
<td></td>
</tr>
<tr>
<td>3.0</td>
<td>2.3</td>
<td>34.6%</td>
<td>8,331</td>
<td>35,593</td>
<td>8.54</td>
<td></td>
</tr>
</tbody>
</table>
3.5 Influence of mean particle size and particle number

As can be seen from the results in Table 3.7, bulk strength and stiffness decreased by 6% and 8% respectively as the number of particles was reduced from 68.6K to 8.3K. However, given the findings from Chapter 3, this decrease in strength could also be attributed to a decrease in packing density seeing as packing porosity and coordination number fell accordingly. If the latter is indeed true, the influence of particle number on bulk strength and stiffness can be presumed to be almost negligible. Interestingly, the bulk response also tends to become gradually more ductile as the particle number is reduced. This is confirmed by the 15% difference in strain at peak strength between the 68.6K and 8.3K packings. Given that it was
concluded that porosity has little influence on ductility, this trend must be due to the change in packing fineness. The trend of increasing ductility as packing fineness decreases is at odds with the observations made by Nitka & Tejchman (2015). However, assuming that increasing mean particle size can be considered equivalent to reducing specimen size, results obtained here agree with DEM results obtained by Sinnaie (2017) and experimental size effect observations made by van Mier, et al. (1997).

Looking at the progression of relative bond breakage shown in Figure 3.14, two items stand out. First, bonds break at a much faster rate in the coarser packing, culminating in 19.6% broken bonds at peak stress compared to merely 14.9% in the fine packing. Again, the increased rate of bond breakage in the coarse sample is likely correlated to an increase in ductility as bond breakage embodies loss of stiffness at the mesoscopic level. The second observation is that bond breakage plateaus at a 32% higher value in the coarse specimen meaning that the latter has lost more of its initial bond structure at the time of ultimate failure. As relative bond breakage can almost certainly be related to a specimen’s internal strain energy, this observation might also help explain why smaller specimens exhibit increased ductility in experimental tests.
3.6 Influence of bond coordination number

The discussions in the previous sections have provided a series of valuable insights by looking at three packing parameters and quantifying their influence on the bulk response independently. However, certain trends, such as the increase of bulk strength and stiffness with increasing packing density, were common across all scenarios. This section investigates those trends by examining the property which relates all bond fabrics together; the coordination number. Note that the coordination number was never a user-specified packing property, but merely a by-product of the other packing parameters. The exact relationship between coordination number and bulk compressive strength and bulk stiffness are shown in Figure 3.15 and Figure 3.16 respectively.
Figure 3.15 Relation between coordination number and ultimate strength.

Figure 3.16 Relation between coordination number and bulk Young’s modulus.

As can be seen from the results in Figure 3.15 and Figure 3.16, there is a strong positive relation between coordination number and bulk compressive
3.6 Influence of bond coordination number

strength and bulk Young's modulus. Specifically, a 12% increase in coordination number led to a 40% increase in $f'_c$ and a 35% increase in $E_{c(0.4)}$. This suggests that geometrical parameters can also be used to calibrate a model to achieve desired bulk properties without adjusting the model's mechanical parameters. In addition, because the relations between bond coordination number and bulk properties are not constrained by a specific packing porosity or packing resolution, bond coordination number is a strong contender to be the principal geometrical bulk calibration parameter.
Chapter 4  Parametric study: Part 2 – DEM mechanical parameters

4.1 Introduction

The second part of the parametric study considers the influence of five carefully selected mechanical parameters. These are the inter-particle and particle-geometry contact friction coefficients; the contact normal-to-shear stiffness ratio and the mean bond tensile and shear strengths. Whilst the approach remains similar as before, the simulations in this chapter are all performed on the identical bond fabric to ensure that the variability caused by the coefficient of variation applied to bond strengths (see Chapter 3) does not interfere with the process of discovering the effects caused by the specific parameters of interest.

4.2 Influence of particle-particle friction

The reference value of the inter-particle coefficient of static friction $\mu_{sp}$ is set at 0.5 based on similar values for typical aggregate materials such as soft rock. In the parametric study $\mu_{sp}$ is varied from 0.1 to 0.75. The resulting bulk properties are summarised in Table 4.1, with corresponding stress-strain profiles presented in Figure 4.1.

<table>
<thead>
<tr>
<th>Particle-particle static friction</th>
<th>Ultimate strength (MPa)</th>
<th>Strain at ultimate strength</th>
<th>Secant elastic modulus (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu_{sp}$</td>
<td>$f_c$</td>
<td>$\varepsilon_c$</td>
<td>$E_{c(0.4)}$</td>
</tr>
<tr>
<td>0.10</td>
<td>48.4</td>
<td>0.160%</td>
<td>37.3</td>
</tr>
<tr>
<td>0.25</td>
<td>49.4</td>
<td>0.159%</td>
<td>37.3</td>
</tr>
<tr>
<td>0.50</td>
<td>48.9</td>
<td>0.155%</td>
<td>37.3</td>
</tr>
<tr>
<td>0.75</td>
<td>49.9</td>
<td>0.162%</td>
<td>37.3</td>
</tr>
</tbody>
</table>
4.2 Influence of particle-particle friction

As expected, the inter-particle coefficient of static friction has no significant influence on the initial stress-strain behaviour. This is because frictional contacts do not mobilise until bond breakage begins. Moreover, the almost identical pre-peak stress-strain curves suggest that even as bonds begin breaking and the specimen begins to lose bulk stiffness at around 50% ultimate strength, the increased contribution from frictional contacts to bulk strength and stiffness is non-existent. The only noticeable difference in behaviour caused by an increase in contact friction is a greater residual post-failure strength which activates at approximately 0.25% strain. Although this sudden residual strength is traditionally not observed in experimental studies, e.g. by van Mier, et al. (1997), it is believed that this discrepancy is caused by differences in macroscopic failure modes between the sharply inclined macro-cracks often seen in experimental studies and the relatively shallow inclined cracks resulting from the DEM simulations shown in Figure 4.2.
4.3 Influence of particle-boundary friction

Experimental studies have shown that by lowering frictional resistance between the sample and the loading plates, strength measurements decrease. In addition, when using extremely low surface-friction plates (e.g. by adding grease), the triaxially-confined boundary zones disappear, causing the specimen to fail by virtue of a vertical tension split (van Mier, et al., 1997).

In the parametric study, the particle-geometry coefficient of friction is investigated for values ranging between 0.0 (infinitely smooth) and 1.0. The resulting stress-strain profiles are shown in Figure 4.3 and a summary of extracted bulk properties is tabulated in Table 4.2.

Figure 4.2 YZ cross-sectional cut showing in-tact (yellow) and broken bonds (black) at 0.3% strain for (a) $\mu_{sp} = 0.10$, (b) $\mu_{sp} = 0.25$, (c) $\mu_{sp} = 0.50$ and (d) $\mu_{sp} = 0.75$. 
4.3 Influence of particle-boundary friction

![Stress vs Strain Graph](image)

**Figure 4.3** Influence of particle-geometry coefficient of static friction.

**Table 4.2** Summary of influence of particle-geometry friction on bulk properties.

<table>
<thead>
<tr>
<th>Particle-geometry static friction</th>
<th>Ultimate strength (MPa)</th>
<th>Strain at ultimate strength</th>
<th>Secant elastic modulus (GPa)</th>
<th>Bulk Poisson’s ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu_{sg}$</td>
<td>$f_c'$</td>
<td>$\varepsilon_c$</td>
<td>$E_{c(0.4)}$</td>
<td>$\nu_{c(0.4)}$</td>
</tr>
<tr>
<td>0.00</td>
<td>46.3</td>
<td>0.147%</td>
<td>37.1</td>
<td>0.198</td>
</tr>
<tr>
<td>0.10</td>
<td>49.9</td>
<td>0.162%</td>
<td>37.3</td>
<td>0.199</td>
</tr>
<tr>
<td>0.25</td>
<td>49.3</td>
<td>0.163%</td>
<td>37.3</td>
<td>0.197</td>
</tr>
<tr>
<td>0.50</td>
<td>49.6</td>
<td>0.157%</td>
<td>37.3</td>
<td>0.195</td>
</tr>
<tr>
<td>1.00</td>
<td>48.9</td>
<td>0.155%</td>
<td>37.3</td>
<td>0.196</td>
</tr>
</tbody>
</table>

The only noticeable difference between responses occurs when there is no static friction at the boundaries. In this friction-less scenario, the initial bulk elastic properties remain the same, however, the values of peak strength and strain at peak strength fall by approximately 6% and 8% respectively. Upon investigating the failure planes, it was discovered that when $\mu_{sg} = 0.0$, bond breakage occurs overwhelmingly at the loading plates as can be seen in Figure 4.4(a). The observable boundary crushing, while too considerable to be realistic, does eventually lead to a tensile splitting macro-crack, indicating that the absence of boundary friction is causing a lack of lateral confinement at the specimen ends (Figure 4.5) as is the case.
4.3 Influence of particle-boundary friction

in experiments. Nonetheless, the extent of boundary damage is greater than what is observed experimentally. Whilst the exact mechanism that occurs near the loading plates is still under investigation, it is believed that it is a function of particle size and that there is a possibility that the choice of not numerically smoothing the specimen boundaries, whilst not influential when selecting $\mu_{sg} > 0$, is in this case causing a disproportionate number of plate-touching particles to slide too easily in the lateral direction resulting in localised bond breakage.

For all cases where $\mu_{sg} > 0$, the quantitative bulk properties are very similar, an observation which agrees with Sinnaie (2017) who determined that the effect of end-friction plateaus at a certain value ($\mu_{sg} = 0.3$ in their case). However, in contrast to what was reported in the aforementioned study, the end-friction coefficient does not influence post-peak ductility. Nevertheless, the failure planes shown in Figure 4.4 indicate that despite not having a noticeable influence on post-peak behaviour, boundary friction does affect the eventual location of the macro-crack, suggesting that the discrepancy between results may be because a different softening law was used in the alternative study.

![Cross-sections of specimens showing bond breakage at 0.3% strain for different $\mu_{sg}$ values](image)

Figure 4.4 Cross-sections of specimens showing bond breakage at 0.3% strain for (a) $\mu_{sg} = 0.0$, (b) $\mu_{sg} = 0.10$, (c) $\mu_{sg} = 0.25$, (d) $\mu_{sg} = 0.50$ and (e) $\mu_{sg} = 1.0$. 

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4.4 Influence of contact normal-to-shear stiffness ratio

In the Timoshenko Beam Bonded Contact Model, the bond’s shear modulus $G_b$ is related to its Young’s modulus $E_b$ and Poisson’s ratio $\nu_b$ such that:

$$G_b = \frac{E_b}{2(1+\nu)}$$  \hspace{1cm} (4.1)

Poisson’s ratio values for most materials fall in the range of 0.1 to 0.4; for this range, given a constant $E_b$, the elastic assumption implies that $G_b$ is constrained to being anywhere between 2.2 to 2.8 times smaller than $E_b$.

In the parametric study, the Poisson’s ratio is actually investigated over a range of -0.4 to 0.5. Note that the physical meaning of a negative bond Poisson’s ratio is that the bonds are assumed to behave as auxetic materials, i.e. when subjected to positive (tensile) axial strains, the transverse strains will actually be positive too (Lakes, 1987). A table summarising the average normal and shear bond stiffness components resulting from the Timoshenko beam calculation is shown in Table 4.3.

Figure 4.5 Indicative normal stress $\sigma_{xx}$ (tension positive) on XZ-plane at $\varepsilon = 0.15\%$ for (a) $\mu_{sg} = 0.0$ and (b) $\mu_{sg} = 1.0$. 

(a) $\mu_{sg} = 0.0$

(b) $\mu_{sg} = 1.0$
Recall that the bond’s Young’s modulus $E_b$ is kept constant at 50 GPa for all simulations.

Table 4.3 Summary of influence of $v_b$ on bond axial and shear stiffness.

<table>
<thead>
<tr>
<th>Bond Poisson's ratio</th>
<th>Bond shear modulus (GPa)</th>
<th>Average bond axial stiffness (MN/m)</th>
<th>Average bond shear stiffness (MN/m)</th>
<th>Normal-to-shear stiffness ratio $k_n/k_s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$v_b$</td>
<td>$G_b$</td>
<td>$k_{n,avg}$</td>
<td>$k_{s,avg}$</td>
<td>$k_n/k_s$</td>
</tr>
<tr>
<td>-0.4</td>
<td>41.7</td>
<td>130</td>
<td>44.1</td>
<td>2.9</td>
</tr>
<tr>
<td>-0.2</td>
<td>31.3</td>
<td>130</td>
<td>38.2</td>
<td>3.4</td>
</tr>
<tr>
<td>0</td>
<td>25.0</td>
<td>130</td>
<td>34.2</td>
<td>3.8</td>
</tr>
<tr>
<td>0.1</td>
<td>22.7</td>
<td>130</td>
<td>32.0</td>
<td>4.1</td>
</tr>
<tr>
<td>0.2</td>
<td>20.8</td>
<td>130</td>
<td>30.3</td>
<td>4.3</td>
</tr>
<tr>
<td>0.4</td>
<td>17.9</td>
<td>130</td>
<td>27.5</td>
<td>4.7</td>
</tr>
<tr>
<td>0.5</td>
<td>16.7</td>
<td>130</td>
<td>26.0</td>
<td>5.0</td>
</tr>
</tbody>
</table>

Table 4.3 shows that the material modulus ratio $E_b/G_b$ does not strictly translate to an equivalent bond stiffness ratio $k_n/k_s$. Moreover, the DEM extracted results indicate that, if the assumption is made that bond force-displacement interactions can be idealised by Timoshenko beam behaviour of typical materials, $k_n/k_s$ values should fall in the range of 4.1 to 4.7, which is significantly larger than some of the ratios used in previous studies, e.g. 2.5 in the case of Sinnaie’s (2017) DEM size effect study. Nonetheless, lower $k_n/k_s$ ratios can still be obtained by selecting negative bond Poisson’s ratios. The influence on stress-strain behaviour is shown in Figure 4.6; DEM bulk properties are shown in Table 4.4.
4.4 Influence of contact normal-to-shear stiffness ratio

Figure 4.6 Influence of normal-to-shear stiffness ratio on stress-strain behaviour.

Table 4.4 Summary of influence of $k_n/k_s$ on DEM bulk properties.

<table>
<thead>
<tr>
<th>Normal-to-shear stiffness ratio $k_n/k_s$</th>
<th>Ultimate strength (MPa) $f_c$</th>
<th>Strain at ultimate strength $\varepsilon_c$</th>
<th>Secant elastic modulus (GPa) $E_{c(0.4)}$</th>
<th>Bulk Poisson's ratio $\nu_{c(0.4)}$</th>
<th>Inclination of failure plane $\theta_{fail}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.9</td>
<td>43.3</td>
<td>0.136%</td>
<td>40.7</td>
<td>0.135</td>
<td>*</td>
</tr>
<tr>
<td>3.4</td>
<td>45.9</td>
<td>0.140%</td>
<td>39.4</td>
<td>0.147</td>
<td>48°</td>
</tr>
<tr>
<td>3.8</td>
<td>46.7</td>
<td>0.147%</td>
<td>38.1</td>
<td>0.188</td>
<td>35°</td>
</tr>
<tr>
<td>4.1</td>
<td>48.4</td>
<td>0.153%</td>
<td>37.7</td>
<td>0.193</td>
<td>39°</td>
</tr>
<tr>
<td>4.3</td>
<td>48.9</td>
<td>0.155%</td>
<td>37.3</td>
<td>0.196</td>
<td>47°</td>
</tr>
<tr>
<td>4.7</td>
<td>50.7</td>
<td>0.170%</td>
<td>36.5</td>
<td>0.204</td>
<td>38°</td>
</tr>
<tr>
<td>5.0</td>
<td>52.0</td>
<td>0.179%</td>
<td>36.0</td>
<td>0.206</td>
<td>35°</td>
</tr>
</tbody>
</table>

* Two macro-cracks were observed - one horizontal and one inclined

As the Poisson’s ratio is increased from -0.4 to 0.5, $k_n/k_s$ increases from 2.9 to 5.0 and the DEM model predicts a gradual decrease in bulk Young’s modulus (down 12%), an increase in bulk ultimate strength (up 20%) and a corresponding increase in strain at peak strength. The bulk Poisson’s ratio also increases by approximately 50%; this means that for $k_n/k_s = 2.9$, the DEM computed bulk Poisson’s ratio is slightly below the typical range for real concrete which is 0.15-0.20
Influence of contact normal-to-shear stiffness ratio

4.4 Influence of contact normal-to-shear stiffness ratio

according to Neville & Brooks (1987), although Mehta & Monteiro (2014) suggest a slightly wider range, namely between 0.10 to 0.20. These observations are in stark contrast to the findings by André, et al. (2012) who concluded that the effect of bond Poisson’s ratio on bulk response is negligible, perhaps showing one of the limitations of the Euler-Bernoulli beam contact model (which was used in that study). Lastly, the angles of the macroscopic failure planes with respect to the horizontal plane were measured to inspect whether a change in relative shear stiffness resulted in a different angle of failure. Although the inclination angle of the failure plane varied between simulations, no clear trend could be identified.

Upon further investigation, the observable macroscopic changes due to changing $k_n/k_s$ can be explained by a combination of factors related to how the average values of the three bond stress components develop in the different scenarios (Figure 4.7).

![Figure 4.7 Progression of average bond stresses, $k_n/k_s = 2.9$ and $k_n/k_s = 5.0$.](image)

As bond normal-to-shear stiffness is increased from 2.9 to 5.0, the following observations are made from the bond average stress curves in Figure 4.7:
4.4 Influence of contact normal-to-shear stiffness ratio

i) As expected, a decrease in shear modulus caused by an increase in $k_n/k_s$ reduces the stiffness of each of the components of the bond fabric. Interestingly, the tensile and shear stiffness components (down 41% and 38% respectively) are affected more by the change than the compressive component is (down 26%).

ii) However, despite a significant reduction in each of the individual stiffness components, the net effect on initial bulk axial stiffness $E_c(0.4)$ is much smaller as shown by Table 4.4. In other words; at the same level of loading strain, internal stresses in the ‘stiff’ specimen are significantly greater than in the ‘flexible’ specimen, yet the resultant stress measured at the boundary plates remains almost identical. The reason for this, as shown by the stress distribution plots of both specimens at $\varepsilon = 0.14\%$ in Figure 4.8, is that although average stresses in the flexible specimen are lower because of a significant reduction of the stresses near the specimen’s centre, compressive stresses near the boundaries are the same in both cases. The Poisson effect caused by an increase in $k_n/k_s$ is leading to larger lateral displacements and lower internal stresses in the flexible specimen without weakening the compressive region near the loading plates. This also proves that merely measuring boundary forces and displacements is not always sufficient to be able to provide a comprehensive picture of the specimen’s internal mechanics.

iii) At peak compressive stress, when $\varepsilon_c$ is 0.14% and 0.18% respectively (dotted lines in Figure 4.7), average internal stresses in both specimens are of comparable magnitude (because bond strengths have remained the same), yet compressive stress measured at the loading plates is 20% greater in the latter scenario.

These last two points provide an interesting proposition for future experimental studies, namely: can concrete be strengthened by optimising the Poisson effect (e.g. by selecting mix materials with high Poisson’s ratios)? Although a prior experimental study by Allos & Martin (1981) found no relationship between bulk Poisson’s ratio and compressive strength, this study only considered Poisson’s
ratio changes by virtue of curing effects and did not consider variation in mix materials. In addition, improved knowledge of the Poisson effect on plain concrete strength and ductility can be beneficial to the future research and design of applications such as lightweight-aggregate concrete (LWA) and steel tube/FRP-confined concrete, where the effects of confinement are already being implemented to significantly improve the strength and ductility of concrete (Han & Xiang, 2017; Dong, et al., 2017).

Figure 4.8 Internal stress distributions ($\sigma_{xx}$ on left and $\sigma_{yy}$ on right) at $\varepsilon = 0.14\%$ (i.e. peak stress for $k_n/k_s = 2.9$); (a) $k_n/k_s = 2.9$ and (b) $k_n/k_s = 5.0$. 
4.5 Influence of bond tensile-to-shear strength ratio

4.5.1 Influence on ultimate compressive strength $f'_c$

The literature currently provides no guidance on how to determine the values of mesoscopic failure criteria. Although most studies agree that bond (or contact) compressive strength should be chosen such that it is seldom the limiting failure mode, the remaining tensile and shear bond failure limits vary greatly between studies.

This section investigates the influence of mean bond tensile strength $S_T$, mean bond shear strength $S_S$ and tensile-to-shear strength ratio $\alpha$ (Equation (4.2)) on macroscopic response to loading by conducting 25 unique simulations with varying input parameters as summarised in Table 4.5.

$$\alpha = \frac{S_T}{S_S} \quad (4.2)$$
4.5 Influence of bond tensile-to-shear strength ratio

Table 4.5 Summary of influence of bond tensile and shear strength on peak values.

<table>
<thead>
<tr>
<th>Run</th>
<th>Tensile-shear ratio</th>
<th>Mean bond tensile strength (MPa)</th>
<th>Mean bond shear strength (MPa)</th>
<th>Bond tensile failures at peak (%)</th>
<th>Bond shear failures at peak (%)</th>
<th>Ultimate strength (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>#</td>
<td>α</td>
<td>ST</td>
<td>SS</td>
<td>B_{b,T}</td>
<td>B_{b,S}</td>
<td>f'_C</td>
</tr>
<tr>
<td>1</td>
<td>0.20</td>
<td>33</td>
<td>165</td>
<td>100%</td>
<td>0%</td>
<td>16.4</td>
</tr>
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<td>94%</td>
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</tr>
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<td>94%</td>
<td>34.4</td>
</tr>
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<td>2%</td>
<td>98%</td>
<td>16.7</td>
</tr>
<tr>
<td>25</td>
<td>6.00</td>
<td>596</td>
<td>99</td>
<td>3%</td>
<td>96%</td>
<td>101.3</td>
</tr>
</tbody>
</table>

Whilst the bulk elastic properties are not displayed for each run, variation between secant elastic moduli $E_{c(0.4)}$ and bulk Poisson's ratio $\nu_{c(0.4)}$ across simulations was less than 5% and 4% respectively. As such, the influence of bond strength on bulk elastic parameters can be assumed to be negligible and the attention is instead directed towards interpreting the values of compressive strength $f'_C$ and bond breakage at peak stress. Figure 4.9 displays the values of relative tensile and shear bond breakage at peak stress for varying ratios of $\alpha$. Notice that because breakage through compression occurs seldom, the sum of broken tensile and shear bonds comprises approximately 100% of total broken bonds in all cases.
4.5 Influence of bond tensile-to-shear strength ratio

Figure 4.9 Relative tensile and shear bond breakage at $f'_{c}$ as a function of $\alpha$.

As indicated by the dotted lines in Figure 4.9, the plot can be divided into three zones: zone A, where $\alpha < 1.5$ and where tensile bond breakage represents more than 85% of total bond breakage; zone C, or $\alpha > 4.0$, where the reverse effect takes place and where shear failure represents more than 85% of bond breakage; lastly, there is an intermediate zone B, identified as $1.5 < \alpha < 4.0$ where both types of failure contribute a considerable amount to total bond breakage. In addition, the point where the two lines intersect, i.e. where $\alpha$ is such that bond breakage is divided equally between tension and shear, corresponds roughly to the ratio between bond Young’s modulus $E_b$ and bond shear modulus $G_b$ which is $2(1 + \nu) = 2.4$ in this case. This means that changing the bond’s Poisson’s ratio will presumably shift the centre of the curve as well as the range of acceptable $\alpha$ values for each zone.

From these results, it was hypothesised that each zone corresponds to a different type of failure mechanism and that the relationship between bond strengths and bulk compressive strength in each zone may be described differently. More specifically, given that pre-peak behaviour in zones A and C are essentially solely governed by bond tensile strength and bond shear strength respectively, it was proposed that the bulk compressive strength in these two zones may be
4.5 Influence of bond tensile-to-shear strength ratio

predicted based uniquely on their respective governing strength parameters. The $f'_c - S_i$ plots shown in Figure 4.10 and Figure 4.11 show the exact relationships between compressive strength and bond strength for zones A and C respectively.

![Figure 4.10](image)

Figure 4.10 – Relation between $f'_c$ and $S_T$ for $\alpha < 1.5$. 

$f'_c = 0.49S_T...$
4.5 Influence of bond tensile-to-shear strength ratio

Figure 4.11 – Relation between $f'_c$ and $S_S$ for $\alpha > 4.0$.

For each zone, there is a strong relation between $f'_c$ and the bond strength parameter which governs bond breakage in that range such that:

$$f'_c = \begin{cases} A_T \times S_T, & \alpha \leq 1.5 \\ A_S \times S_S, & \alpha \geq 4.0 \end{cases}$$

(4.3)

where $A_T$ and $A_S$ are the slopes of the lines which in this case are 0.49 and 1.02 respectively, although the exact values will vary depending on the other parameters (mostly packing parameters and bond Young’s modulus $E_b$) used. Interestingly, $A_S \approx 2 \cdot A_T$ in this case (recall this is roughly the inverse of the ratio of $E_b$ to $G_b$), suggesting that there may be a more fundamental relationship between bond failure criteria and corresponding bulk compressive strength which takes into account the effect of bond stiffnesses in addition to what is presented here. For zone B, the approach taken to relate bond strength parameters to $f'_c$ was to assume that the ultimate strength can be split up into a tensile and a shear ‘contribution’. The coefficients for each contribution depend on the value of $\alpha$ as shown in Figure 4.12 and can be determined by linearly interpolating between fixed values which were found iteratively. Thus, the contributions from the tensile and shear components can
be combined with the linear relationships earlier to calculate the compressive strength, such that for zone B:

\[ f'_c = \beta [C_T A_T S_T + C_S A_S S_S], \qquad 1.5 < \alpha < 4.0 \quad (4.4) \]

where \( A_T \) and \( A_S \) are the constants determined earlier and \( C_T \) and \( C_S \) are the tensile and shear contribution coefficients given by:

\[ C_T = 1.22 - 0.28 \times \alpha \quad (4.5) \]

\[ C_S = 1 - C_T \quad (4.6) \]

and \( \beta \) is a reduction factor to account for the combined effect, taken as 0.85.

![Figure 4.12 Tensile and shear contribution coefficients to compute \( f'_c \) when \( \alpha \) is in zone B.](image)

Table 4.6 shows how the values of \( f'_c \) calculated using Equations (4.3) and (4.4) compare with DEM computed values for all the simulations.
Influence of bond tensile-to-shear strength ratio

Table 4.6 Comparison of $f'_e$ calculated using Equations (4.3) & (4.4) and DEM computed values of $f'_e$ (from Table 4.5).

<table>
<thead>
<tr>
<th>Zone</th>
<th>Run</th>
<th>Ultimate strength DEM (MPa)</th>
<th>Ultimate strength, Eqs. (4.3) &amp; (4.4)</th>
<th>Relative error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$f'_e$</td>
<td>$f'_{e,eq}$</td>
<td>$E_r$</td>
</tr>
<tr>
<td>A</td>
<td>1</td>
<td>16.4</td>
<td>16.2</td>
<td>1%</td>
</tr>
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<td></td>
<td>2</td>
<td>50.9</td>
<td>48.7</td>
<td>4%</td>
</tr>
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<td>3%</td>
</tr>
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<td>25</td>
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Table 4.6 shows that Equations (4.3) and (4.4) are able to accurately predict $f'_e$ values for a wide range of tensile and shear bond strengths. However, it should be noted that in their current formulation, the equations are only valid for a unique set of packing and mechanical parameters, meaning that a change in these parameters would require generating a different set of calibration data to obtain the necessary coefficients. As such, the next step in enhancing these equations would be to unify all existing calibration relationships such that given any set of input parameters, there
will exist a set of equations able to accurately predict all meso and bulk properties regardless of the contact model or software used.

### 4.5.2 Influence on softening and fracture behaviour

This section uses simulations 3, 15 and 21 from zones A, B and C respectively as example scenarios to study the influence of bond strength on post-peak behaviour given that they all share similar values of $f_{c'}$. The key bulk properties shown in the previous section are summarised again in Table 4.7 for convenience. In addition, stress-strain curves for each of the three simulations are presented in Figure 4.13 and damage plots immediately after the formation of macro-cracks (as stress-strain curve begins to plateau) are displayed in Figure 4.14.

Table 4.7 Simulations selected to study post-peak behaviour (originally from Table 4.5).

<table>
<thead>
<tr>
<th>Run</th>
<th>Tensile-shear ratio</th>
<th>Mean bond tensile strength (MPa)</th>
<th>Mean bond shear strength (MPa)</th>
<th>Bond tensile failures at peak (%)</th>
<th>Bond shear failures at peak (%)</th>
<th>Ultimate strength (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>#</td>
<td>$\alpha$</td>
<td>$S_T$</td>
<td>$S_S$</td>
<td>$B_{b,T}$</td>
<td>$B_{b,S}$</td>
<td>$f_{c'}$</td>
</tr>
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<td>3</td>
<td>0.50</td>
<td>66</td>
<td>132</td>
<td>98%</td>
<td>2%</td>
<td>34.7</td>
</tr>
<tr>
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<td>165</td>
<td>33</td>
<td>6%</td>
<td>94%</td>
<td>34.4</td>
</tr>
</tbody>
</table>
4.5 Influence of bond tensile-to-shear strength ratio

Figure 4.13 Influence of bond strength ratio $\alpha$ on stress-strain behaviour.

Figure 4.14 Damage plots taken upon formation of macro-crack for (a) $\alpha = 0.5$, (b) $\alpha = 3.0$ and (c) $\alpha = 5.0$.

Although Figure 4.13 only shows stress-strain curves for three values of $\alpha$, the stress-strain profiles for Run 3, Run 15 and Run 21 are found to adequately
represent all other tensile-dominant, mixed failure, and shear-dominant simulations respectively. The general stress-strain behavioural trends for each zone can be described as follows:

i)  $\alpha < 1.5$ or tensile-dominant:
   - Low ductility and highly localised damage development leading up to peak stress;
   - Rapid breakage of bonds and subsequent loss of strength post-peak (see Figure 4.15);
   - Formation of inclined macro-crack with maximum angle greater than 35° w.r.t. the horizontal plane.

ii) $1.5 < \alpha < 4.0$ or mixed failure:
   - Moderate ductility and spread out damage progression leading up to peak stress;
   - Moderate rate of bond breakage and residual strength post-peak;
   - Formation of one or two horizontal macro-cracks.

iii) $\alpha > 4.0$ or shear-dominant:
   - Moderate ductility leading up to peak stress;
   - High post-peak residual stress;
   - Formation of one or two horizontal macro-cracks.
4.5 Influence of bond tensile-to-shear strength ratio

Furthermore, plotting the progression of average bond stresses (Figure 4.16) shows that the main reason for the rapid loss of post-peak strength in the brittle specimen can be attributed to the fact that as tensile bonds begin to break (average tensile stress plateaus), there is a significant reduction in the average compressive stress in the specimen which in turn leads to a lower bulk stress measured at the boundary plates. This suggests that when future development of the EBPM considers adding mesoscopic softening parameters to improve model ductility, it may be necessary to calibrate initial bulk loss of stiffness using a compressive softening parameter, whereas bulk post-peak softening will be more sensitive a tensile component and that these are not necessarily described by the same parameter or damage theory.

Figure 4.15 Influence of $\alpha$ on relative bond breakage at peak stress and upon formation of macro-crack.
4.5 Influence of bond tensile-to-shear strength ratio

Figure 4.16 Influence of $\alpha$ on progression of average bond stresses.

The angle of the macroscopic failure plane corresponding to the different categories of governing bond failure is believed to be related to the orientation of maximum stresses inside the specimen. The directions of principal stress $\sigma_1$ in a typical simulation (Run 6) shown in Figure 4.17 show that the maximum internal stresses are oriented arbitrarily along the XY-plane (no vertical arrows). Therefore, bonds carrying the greatest tensile stresses will be predominantly oriented horizontally whereas bonds subjected to the greatest shear stresses will mostly be vertically oriented. This is confirmed to a certain extent by plotting the bonds with above-average tensile and shear stresses at the same time step as is displayed in Figure 4.18.
4.5 Influence of bond tensile-to-shear strength ratio

Figure 4.17 Vectors of principal stress $\sigma_1$ directions looking at the (a) XZ-plane and (b) YZ-plane when loading is at 40% $f_c'$.

Figure 4.18 Orientation of bonds for which (a) $\sigma_S > 1.5\sigma_{S,avg}$ and (b) $\sigma_T > 1.5\sigma_{T,avg}$ when loading is at 40% $f_c'$. 
These observations suggest that when bond breakage occurs predominantly through tension, the majority of breakage occurs in horizontally oriented bonds and that the resulting macro-crack propagates perpendicular to these broken bonds leading to an inclined failure plane. In contrast, when shear dominates, bond breakage will predominantly affect vertically oriented bonds and as such the resulting macro-crack propagates radially leading to the horizontal cracks observed in Figure 4.14(b) and Figure 4.14(c).

Given that horizontal macro-cracks are rarely, if ever witnessed in experimental studies, reasoning dictates that tensile-dominant bond breakage should be chosen as the mesoscopic mechanism to represent concrete and that the tensile-shear bond strength ratio should be chosen accordingly. The importance of understanding the underlying damage mechanisms and the mesoscopic parameters that cause these cannot be understated. Looking only at the bulk stress-strain graphs shown in Figure 4.13, one might be inclined to argue that the shear-dominant case better simulates a typical concrete specimen given that its stress-strain curve agrees better with curves shown in design codes, yet based on current experimental evidence of fracture phenomena, the opposite is true. Nevertheless, additional studies combining DEM with experimental techniques such as μCT-imaging should be conducted to provide more clarity on this.

4.5.3 Predicting crack propagation

Using DEM simulation results in combination with P4’s post-processing capabilities, it is possible to closely monitor the formation and propagation of micro- and macro-cracks. Figure 4.19, Figure 4.20 and Figure 4.21 show the progression of bulk stress, local damage and internal stress respectively for ‘Run 3’ ($\alpha = 0.5$ from the previous section) as it is subjected to increasing strain.
4.5 Influence of bond tensile-to-shear strength ratio

Figure 4.19 Stress-strain curve of ‘Run 3’ (reproduced from Figure 4.13) showing points of loading for plots in Figures 4.20 and 4.21.

Figure 4.20 Local particle damage $D_m$ at (a) $\epsilon = 0.92\epsilon_c$ (corresponds to $0.95f'_c$), (b) $\epsilon = \epsilon_c$ and (c) $\epsilon = 1.07\epsilon_c$
4.5 Influence of bond tensile-to-shear strength ratio

Figure 4.21 Normal stress $\sigma_{xx}$ (tension positive) at (a) $\varepsilon = 0.92\varepsilon_c$ (corresponds to $0.95f'_c$), (b) $\varepsilon = \varepsilon_c$ and (c) $\varepsilon = 1.07\varepsilon_c$

As shown by Figures 4.19 and 4.20, macro-crack formation occurs immediately following peak stress. In addition, although the macro-crack has not yet developed fully at peak, there are already signs indicating where the macro-crack is likely to form as can be seen from the damaged zones in the upper region near where the crack eventually forms. In fact, the damage in this zone can be traced back to as early as when the specimen is subjected to 95% of $f'_c$ (Figure 4.20(a)).

Unlike the damage plots which show the exact location of where cracks occur, the normal stress plots in Figure 4.21, which are taken at the same time steps, show the general regions of high tensile and compressive stresses. By comparing Figures 4.20 and 4.21, it can be seen that the area where the crack eventually develops corresponds to the zone where tensile stresses are highest. Again, this can be noticed as early as $0.95f'_c$ on the stress-strain curve. Post-peak, however, the specimen's internal stress distribution suddenly changes (Figure 4.21(c)) following the formation of a macro-crack which causes stresses to be redistributed as the original tensile zone is no longer capable of resisting the significant forces imposed by the loading plates.

The results obtained in this section concerning the timing of when micro- and macro-crack formation occurs in plain concrete specimens agree with prior experimental and numerical studies (Kirane, et al., 2014). On the topic of predicting
4.5 Influence of bond tensile-to-shear strength ratio

the location of crack formation, the observations made here show that DEM offers an interesting alternative to traditional structural health monitoring experimental methods such as wavelet packing analysis (Lei, et al., 2017) and digital image correlation (Fayyad & Lees, 2017). Although the location of crack formation could not be identified as early as 0.6$f'_{fc}$ as has been the case in other studies (Lei, et al., 2017), there is reason to believe that subsequent modelling efforts may improve this feature of the model. In fact, due to the recentness of P4’s compatibility with the bond model, post-processing of damage predictors at the time of conducting the study was limited to the properties shown in Figures 4.20 and 4.21. However, future studies may consider monitoring other local descriptors such as ‘bond closeness to failure’, i.e. bond stress divided by bond strength, or conventional continuum kinematic properties such as internal strains and displacements.
Chapter 5   Concluding remarks

5.1 Summary

Through the medium of a comprehensive parametric investigation, this thesis has identified concrete’s key mesoscopic descriptors, examined their interdependent relationships and quantified their influence on concrete’s essential macroscopic behavioural properties. A unifying set of equations which relate tensile and shear failure parameters to ultimate compressive strength are proposed and have been shown to be able to accurately predict DEM-computed bulk mechanical properties.

First, a robust numerical methodology which accurately embodies the displacement-controlled uniaxial compression test was set up and verified by ensuring processed simulation results were both correct and sensible. In addition, a full set of results concerning the model’s geometrical input parameters was obtained by means of a collective research effort to establish confidence that the discrete bond fabric chosen to depict the concrete specimen used for parametric testing was represented in an optimal way. Furthermore, the aforementioned results showed that the investigated geometrical input parameters are closely related to macroscopic behaviour and that said parameters may be used as effective DEM bulk calibration parameters in future studies. Lastly, a comprehensive study of the model’s meso-mechanical parameters, including contact friction, stiffness, and strength was conducted to critically interrogate how these parameters affect the mechanical phenomena which occur at the mesoscopic level as concrete is loaded to compressive failure. New approaches to the representation, analysis, and interpretation of discrete simulation data are presented, discussed, and used to establish and quantitatively describe the apparent relationships between mesoscopic stiffness and damage properties and bulk ultimate compressive strength.
5.2 Conclusions

5.2.1 Initial particle packing & bond fabric

I. Bond fabric coordination number is closely correlated to bulk compressive strength $f'_c$ and Young's modulus $E_{c(0.4)}$. A 12% increase in coordination number leads to a 40% increase in $f'_c$ and a 35% increase in $E_{c(0.4)}$, indicating that this packing property can be used as an effective bulk calibration parameter.

II. A reduction in packing porosity $n$ leads to a proportional rise in compressive strength $f'_c$ and Young's modulus $E_{c(0.4)}$. However, variation in packing porosity does not influence stress-strain behaviour when it is normalised w.r.t. peak stress and corresponding strain. Hence, a range of porosities can be used as long as the chosen value is kept constant throughout any subsequent calibration or scaling procedure.

III. By introducing a user-specified mechanical coefficient of variation, the model is able to accurately predict variability at the bulk level in terms of bulk Young's modulus $E_{c(0.4)}$ but underpredicts the variation in compressive strength $f'_c$ by approximately 50% when compared to experimental observations reported in the literature.

IV. A rise in bond fabric heterogeneity by means of increasing the discrepancy between maximum and minimum particle radii leads to more rapid development and greater spatial distribution of damage pre-peak which in turn results in a rise in ductility.

V. The EBPM is capable of capturing size effect features consistent with other experimental and numerical studies such as greater pre-peak ductility and a rise in post-peak residual strength as particle size is decreased. On the other hand, the inverse relation between reducing particle size and bulk compressive strength $f'_c$ was not observed.
VI. Increasing packing and bond fabric heterogeneity by switching from normal to uniform particle size distributions has a minimal effect on bulk properties as compared to other parameters investigated in this study.

VII. An exhaustive parametric investigation of the bond fabric parameters has shown that whilst certain parameters are able to marginally affect bulk loss of stiffness, macroscopic ductility predicted by the DEM model remains significantly lower than what is suggested by empirical models based on experimental results. Producing an adequate strain-softening response is evidently a weakness of the model, however, it cannot be solved by adjusting bond fabric parameters solely as this is only part of the model definition.

5.2.2 DEM Mechanical parameters

I. Assuming bonded contacts can be represented mechanically by Timoshenko beam behaviour of typical structural materials, the contact (or bond) normal-to-shear stiffness ratio $k_n/k_s$ should fall in the range of 4.1 to 4.7, which is higher than the ratio used in a number of prior studies. To obtain lower $k_n/k_s$ ratios, bonds can be assumed to possess negative Poisson’s ratios.

II. Increasing $k_n/k_s$ from 2.7 to 5.0 causes a Poisson effect which increases lateral displacements but lowers internal stresses and ultimately leads to a 12% decrease in bulk Young’s modulus $E_{c(0.4)}$, a 20% increase in bulk compressive strength $f'_c$, and a 50% increase in bulk Poisson’s ratio $\nu_{c(0.4)}$.

III. Despite similar pre-peak bulk stress-strain curves, internal stresses leading up to peak strength vary significantly as $k_n/k_s$ is increased, proving the point that describing a specimen’s behaviour merely by the forces and displacements measured at the loading plates can fail to capture important mechanical effects.

IV. The relation between bond failure limits and bulk compressive strength $f'_c$ is highly sensitive to the ratio between the tensile and shear components of the failure criteria (defined as $\alpha$ in this study). For a reference $k_n/k_s$ value of 4.3 used in this study, the following observations are made: when $\alpha < 1.5$, tensile failure governs and $f'_c$ can be predicted based solely on the value of tensile strength $S_T$ by the equation $f'_c = 0.49S_T$; when $\alpha > 4.0$, shear failure governs...
and \( f'_c \) can be related directly to shear strength \( S_s \) where \( f'_c = 1.02S_s \); for \( 1.5 < \alpha < 4.0 \), both \( S_T \) and \( S_S \) must be considered.

V. Due to the orientation of internal stresses in response to compressive loading, macroscopic post-peak behaviour and the inclination of the eventual macro-crack is dependent on the dominant mesoscopic failure mode. When tensile failure dominates, damage develops locally, macroscopic pre-peak ductility is low, and upon reaching peak compressive stress \( f'_c \), an inclined crack forms leading to rapid loss of strength. In contrast, in mixed failure scenarios and when shear dominates, damage develops and spreads at a faster rate, ductility is significantly greater, and macroscopic fracture is characterised by one or two horizontal cracks.

VI. Given that horizontal cracking is uncommon in typical concrete uniaxial testing based on prior experimental evidence, the recommendation is made that bond failure criteria should be chosen such that tensile failure is dominant (\( \alpha < 1.5 \) in this study).

VII. By closely monitoring local mechanical descriptors, the DEM model is able to accurately predict the timing of micro- and macro-crack formation. In addition, the model is able to identify zones which are prone to cracking as early as when loading is at 95\% \( f'_c \).

VIII. The inter-particle coefficient of static friction \( \mu_{sp} \) has no influence on pre-peak stress-strain behaviour. However, the effect on post-peak residual strength is significant: increasing \( \mu_{sp} \) from 0.10 to 0.75 results in a 150\% greater residual strength upon formation of a macro-crack.

IX. The EBPM is able to qualitatively capture the effects of loading plate friction by considering a particle-geometry coefficient of static friction \( \mu_{sg} \). When the loading plate is infinitely smooth, the lack of end confinement leads to the formation of a vertical splitting macro-crack similar to previously reported experimental observations. For all values of \( \mu_{sg} \) greater than 0.0 macroscopic failure planes vary but stress-strain behaviour remains unchanged.
5.3 Recommendations for future work

This thesis identifies, examines, and quantitatively describes the relations between concrete's key mesoscopic parameters and its response to compressive loading. There are, naturally, areas which require further investigation and opportunities to enhance the model and its applicability to industrial and research problems. The identified areas of further study are:

I. The desirable consequences of an increased Poisson effect on DEM response identified in Chapter 4 provide an interesting research question for prospective experimental studies which aim to enhance the design of high-strength and lightweight-aggregate concrete mixes. Moreover, given that the extent to which maximum stress orientations and resulting cracking phenomena fluctuate by virtue of the Poisson effect has not been quantified, combined DEM – experimental micro-facture studies would provide an opportunity to monitor representative crack development and relate these to DEM parameters.

II. The model’s ability to identify and predict micro- and macro-cracking should be revisited once additional post-processing tools become available. Specifically, it would be interesting to monitor each bond’s displacements, strains, and ‘closeness to failure’ as a specimen is loaded to failure. In addition, the model’s predictive capabilities suggest that there is potential for the model to be used in conjunction with experimental monitoring techniques such as digital image correlation (DIC) to aid in the damage protection of structures.

III. The exact equations and coefficients relating bond failure criteria to compressive strength presented in Chapter 4 will presumably only be valid for a specific set of reference parameters. However, as discussed in the same chapter, it is strongly believed that there exists a more fundamental relationship between all meso-parameters and the resulting bulk mechanical properties. As such, subsequent studies should aim to unify the existing calibration relationships presented in this thesis and cultivate a set of prediction equations which are independent of the parameters, contact model, or software used.
IV. Because of the linear elastic constitutive model and the brittle damage law, the EBPM contact model tends to underpredict macroscopic ductility. Future development of the model should, therefore, consider implementing carefully chosen additional softening parameters.

V. Although the elastic portion of the model has been shown to be scale-invariant, questions surrounding the effect of scaling on post-peak behaviour and how this relates to the 'size effect' observed in real concrete remain unanswered and should be investigated in more detail.
References


Particle Analytics Ltd, n.d. Particle Analytics Documentation, Edinburgh: s.n.


