COMPUTATIONAL TECHNOLOGY FOR DAMAGE AND FAILURE ANALYSIS OF QUASI-BRITTLE MATERIALS

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Abstract

The thesis presents the development and validation of novel computational technology for modelling and analysis of damage and failure in quasi-brittle materials. The technology is demonstrated mostly on concrete, which is the most widely used quasi-brittle material exhibiting non-linear behaviour.

Original algorithms and procedures for generating two-dimensional (2D) and three-dimensional (3D) heterogeneous material samples are developed, in which the mesoscale features of concrete, such as shape, size, volume fraction and spatial distribution of inclusions and pores/voids are randomised. Firstly, zero-thickness cohesive interface elements with softening traction-separation relations are pre-inserted within solid element meshes to simulate complex crack initiation and propagation. Monte Carlo simulations (MCS) of 2D and 3D uniaxial tension tests are carried out to investigate the effects of key mesoscale features on the fracture patterns and load-carrying capacities. Size effect in 2D concrete is then investigated by finite element analyses of meso-structural models of specimens with increasing sizes. Secondly, a 3D meso-structural damage-plasticity model for damage and failure analysis of concrete is developed and applied in tension and compression. A new scheme for identifying interfacial transition zones (ITZs) in concrete is presented, whereby ITZs are modelled by very thin layers of solid finite elements with damage-plasticity constitutive relations. Finally, a new coupled method named non-matching scaled boundary finite element-finite element coupled method is proposed to simulate crack propagation problems based on the linear elastic fracture mechanics. It combines the advantage of the scaled boundary finite element method in modelling crack propagation and also preserves the flexibility of the finite element method in re-meshing. The efficiency and effectiveness of the developed computational technology is demonstrated by simulations of crack initiation and propagation problems.

Keywords: Quasi-brittle material, Concrete, Random generation and packing, Crack propagation, Size effect, ITZ, CZM, Damage-plasticity, SBFEM, Monte Carlo simulation
Declaration

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List of publications

Journal papers:


Conference papers:


1. Introduction

CHAPTER ONE

Introduction

1.1 Background

Engineering materials contain defects at multiple length scales, from nano-, through micro-, to meso-scale. Under external loadings, these small-scale defects may develop into macro-scale cracks. The initiation and propagation of cracks in structural components challenge their integrity and the safe exploitation of entire structures. Therefore, understanding crack propagation behaviour by laboratory experiments and numerical simulations has attracted tremendous attention in last decades (e.g. [1-7]). The knowledge of cracks and their behaviour under stress can be invaluable in increasing the longevity of fractured mechanical systems. Accurate stress analysis that reliably estimates the severity of cracks and their need for attention can assist in maintenance programs and reduce financial overheads by the prediction and prevention of otherwise potentially catastrophic failures. This is of particular importance in industries that operate under low factors of safety or with tight profit margins [8].

Physical processes range significantly in complexity [9-14]. Certain relatively simple problems may be described adequately by simple mathematical equations or physical experiments [15, 16]. Other processes, such as the material response of a composite structure, are complicated enough that analytical solutions are not sufficient, efficient or even possible. For example, the mechanical response of concrete subjected to different loadings is dictated by complex geometries and random material microstructures. In such cases, numerical approximation techniques provide the only efficient and economically viable way to approach a safe solution [17]. And these challenges motivated the author to proceed with the development and assessment of new computational technology for damage and failure analysis of quasi-brittle materials. But the demonstrations in this thesis are mostly focused on concrete where sufficient data is available for material parameters and result validations. Concrete is a typical quasi-brittle material composed of multiple phases including aggregates, mortar, interfacial transition zones (ITZs) between the
aggregates and mortar, and various defects such as pores/voids and weak inclusions. The observed mechanical behaviour of concrete is a result of the multiple failure mechanisms operating at a range of different physical scales, and the numerical modelling for interpreting the complex crack initiation and propagation on concrete has gained increasing attention in recent years [18-24].

1.2 Aims and objectives

The aims of this research are to develop and validate practical and efficient numerical analysis tools for fracture modelling in quasi-brittle materials. The efforts are focused on developing computational technology for fracture modelling, reproducing the macroscopic behaviour of concrete specimens, both in terms of stress-strain, toughness-strain curves and in terms of fracture initiation, bridging, branching, propagation, cracking patterns and other phenomena observed. To achieve the aims, the work involves following challenging objectives:

1. To develop a numerical tool for generating both two-dimensional (2D) and three-dimensional (3D) heterogeneous models, in order to study concrete at the mesoscopic level. As the pores/voids may have adverse effects on the damage and fracture behaviour of quasi-brittle materials, they are necessary to be included in the generated geometric models;

2. To develop automatic generation of finite element meshes of heterogeneous materials, including the identification of both zero-thickness interface elements and thin layers of solid elements for ITZs, required for statistical analysis of a series of specimens with different inclusion spatial distributions;

3. To validate the 2D and 3D models against available experimental data of concrete damage and fracture under different loading conditions;

4. To perform size effect study on mesoscopic concrete without notches, and based on the results to propose proper size effect laws;

5. To improve the numerical modelling efficiency and accuracy by taking advantages of different numerical methods, e.g. finite element method (FEM) and scaled boundary finite element method (SBFEM), for fracture modelling problems.

1.3 Thesis outline

This thesis deals with developing computational technology for damage and failure analysis of quasi-brittle materials. Three different numerical models, namely,
cohesive zone model, damage-plasticity model and coupled finite element (FE)-scaled boundary finite element (SBFE) model are proposed for fracture modelling of quasi-brittle materials. Intersection and overlap checking algorithms for randomly distributed 2D circular, elliptical and polygonal, 3D spherical, ellipsoidal and polyhedral inclusions and pores/voids are proposed. Independent software named heterogeneous material generator (HMG) is developed for generating a variety of heterogeneous materials, such as concrete, fibre reinforced composites, cement paste, graphite, etc. The ANSYS Parametric Design Language (APDL) programs in combination with ANSYS batch processing [25] are developed to automatically generate 2D and 3D meshes for a large number of heterogeneous specimens required for Monte Carlo simulations. In-house programs for inserting cohesive interface elements (CIEs) between solid finite elements and identifying the solid elements of ITZs for both 2D and 3D heterogeneous material are developed. Extensive Monte Carlo simulations of damage and failure, and size effects on concrete are conducted based on cohesive zone model and damage-plasticity model. A non-matching FE-SBFE coupled method for simulating crack propagation is proposed and validated with experimental data.

The contents of each chapter are briefly described in the following:

Chapter 1 provides a general introduction to the research background, aims and objectives and outline of the thesis;

Chapter 2 includes an overview of the damage and failure modelling of concrete. Concrete modelling at different scales, alternative schemes for ITZ representation, 2D and 3D modelling are first reviewed. Then the recent techniques to characterize concrete heterogeneity, such as random distributed model, random field model, lattice representation and image based model, are discussed. The numerical models for implementing simulations and size effect theories are also summarized;

Chapter 3 presents the Monte Carlo simulations of mesoscale fracture modelling of concrete with random aggregates and pores. It includes numerical specimen generation and cohesive zone modelling of heterogeneous concrete in 2D;

Chapter 4 describes the main results from size effect study by Monte Carlo simulations of mesoscale fracture of concrete with random aggregates and pores. Size effects on strength and toughness in 2D concrete specimens without notches are investigated under uniaxial tension with a few size effect laws suggested;
Chapter 5 extends the 2D Monte Carlo simulations to 3D modelling of heterogeneous concrete specimens. The main results show a good agreement with the experimental data, and the study provides valuable insights for employing numerical models for fracture analysis in order to ultimately guide the design of better concrete with enhanced stress, fracture toughness and ductility;

Chapter 6 gives a thorough comparison between the 2D and 3D modelling in terms of geometrical representation, strength, toughness and cracking patterns, etc;

Chapter 7 develops a 3D meso-structural damage-plasticity model for damage and failure analysis of concrete in tension and compression. An alternative scheme of modelling ITZs as thin layers of solid elements with damage-plasticity constitutive relation is presented;

Chapter 8 proposes a novel method coupling FEM and SBFEM for linear elastic crack propagation modelling, and a few plane problems are modelled to validate the new method;

Chapter 9 summarises the conclusions of the work and perspectives for future research.

1.4 References


A Review on Damage and Failure Modelling of Concrete

Concrete is a widely used construction material characterized by non-linear behaviours, and its mechanical response strongly associates with the multiple phases within the heterogeneous structure. Concrete is a composite material which is basically made up of cement, aggregates and water, and at mesoscale it is conventionally represented as pores/voids, mortar (cement and fine aggregates), coarse aggregates embedded in mortar and ITZs between mortar and aggregates. Due to the multi-phase composition and quasi-brittle mechanical behaviour over the nano-, micro-, meso- and macro-scales [1, 2], modelling of concrete for structural engineering analysis has been a challenge for several decades, and up to now many details, such as strain softening, micro-crack propagation, failure mechanisms and size effect, etc are still far from being fully understood.

2.1 Concrete modelling at various scales

In numerical simulations of concrete, there are basically three levels of observation: macroscale, mesoscale and microscale. Concrete is normally assumed to be an isotropic and homogeneous material at the macroscale when the global response is of primary interest [3]. It is computationally economical to model concrete at the macroscale with homogenized material properties, and such approaches are commonly used by structural engineers for a wide range of applications, see for example [4-6]. At the mesoscale, concrete is usually regarded as a composite material consisting of coarse aggregates, mortar with embedded fine aggregates, and ITZs [1, 7, 8]. Modelling concrete at this scale permits a more direct description of the material heterogeneity and then allows for a more realistic prediction of the development of damage within the multi-phase material (e.g. [9, 10]). At the microscale, mortar is subdivided into fine aggregates and hardened cement paste, and the cement paste is largely composed of unhydrated cement particles, hydration products and capillary pores [11]. It is the topology of this microstructure that controls the behaviour of concrete at the longer meso- and macro-scales.
Concrete is generally used in large size structures, and a mesoscopic level of observation allows a detailed description of the majority of the important concrete constituents, e.g. aggregates, mortar, pores/voids and ITZs [12, 13]. In order to investigate the damage and failure of this heterogeneous quasi-brittle material, analysis at the mesoscale rather than the macroscale or microscale becomes most practical and useful for evaluating the mechanical behaviour of concrete, and will be the main topic of this study.

2.2 Alternative schemes for interfacial transition zones (ITZs)

ITZs are the specific zones in the vicinity of coarse aggregates, which are formed between mortar and aggregates. Many experimental and numerical techniques including the newly developed nano-indentation have been employed to measure the mechanical properties of ITZs, while the properties are still not fully understood due to the complex microstructures [14, 15]. It is generally recognized that ITZs play a critical role in the concrete fracture process, and are mechanically weaker than mortar and aggregates due to the presence of a large amount of pores and the gradient of the porosity from mortar to aggregate surface [1, 7, 16]. Therefore, an appropriate representation of the ITZs is essential in mesoscale modelling.

It is found in Garboczi and Bentz [17] that the thickness of ITZs is about 10-30 μm, thus modelling such thin layers of elements in a FE model may lead to numerical difficulties. Instead, zero-thickness cohesive interface elements (CIEs) seem to be a rational choice [18]. However, the typical constitutive laws designed for CIEs are primarily for modelling interface fracture, and thus may not fully represent the shear response and the interaction between shear and compression. In order to accommodate general loading conditions, specific cohesive models are required to incorporate the mechanism that the shear strength is highly dependent on the normal stress at the interfaces [19-21]. As an alternative choice, thin layers of solid finite elements equipped with damage-plasticity constitutive behaviour are used to represent ITZs [7, 22]. By employing damage-plasticity constitutive laws to the thin layers of ITZs, the difficulties associated with typical cohesive zone models are avoided, but at the expense of large numbers of elements especially in 3D. Moreover, some numerical modelling even assumes perfect bonding between aggregates and mortar, and thus neglects the existence of the ITZs [13, 23].
2.3 2D and 3D modelling

There are basically two aspects for mesoscale modelling of concrete, namely, the morphological representation of the material heterogeneities, and the implementation of numerical simulations on mechanical behaviours. Due to the challenging task of generating 3D specimens taking into account most of the key parameters, such as shape, size, gradation, volume fraction and spatial distribution of phases, and the constraints of computational power, most of the studies found are still applied in 2D. Lopez et al. [24, 25] proposed a meso-mechanical model using fracture-based zero-thickness interfaces to analyze 2D concrete specimens under uniaxial and biaxial loading. Tu and Lu [16] generated 2D concrete specimens with polygonal aggregates for static and dynamic analysis.

Although the majority of the research on mesoscale modelling of concrete has been focused on 2D, several 3D meso-structural analyses have been performed to predict the damage and failure of concrete. Caballero et al. [19, 26] generated 3D numerical concrete with polyhedral aggregates using Voronoi tessellation method, and effectively reported concrete behaviour under tension and compression. Kim and Abu Al-Rub [7] proposed a coupled plasticity-damage model and used it to simulate concrete with spherical aggregates under tension.

2.4 Concrete heterogeneity characterization and representation

There are, basically, two approaches to generating a meso-structural model of concrete: the parameterization modelling technique and the numerical image processing technique. In the parameterization modelling technique, direct characterization, e.g. random distributed model, and indirect characterizations, e.g. random field model and lattice representation, are used. In the numerical image processing technique, a high-resolution camera or X-ray computed tomography (XCT) scanner is used to capture digital images of the concrete meso-structure. A more detailed and extensive review is presented as follows.

2.4.1 Random distributed model

Monte Carlo sampling [12, 13] and Voronoi tessellation [19, 26] are the two main methods for generating random distributed models. In the Monte Carlo sampling method, the different phases in the concrete such as the mortar, aggregates and
interfaces are explicitly modelled with inclusions generated from a certain size distribution and then placed into the concrete specimen in such a way that there is no intersection or overlap between them (see Fig. 1). In a typical Voronoi tessellation method, a regular distribution of points is first generated in a space by a random function, inclusions are then generated by shrinking each triangle or tetrahedron followed by connecting the centres of Delaunay triangular or tetrahedral mesh. Realistic stress displacement relations and complex crack patterns were successfully simulated using both models [13, 26].

![2D samples](image1). (a) 2D samples (After [27])

![3D samples](image2). (b) 3D samples (After [28])

Fig. 1. Randomly generated numerical concrete samples

For modelling concrete at mesoscale, many researchers, such as Beddow and Meloy [29], Kim and Abu Al-Rub [7], Xu et al. [30] assumed aggregates to be circular in 2D, and Bazant et al. [31], Man et al. [32] and Wriggers et al. [13] generated spherical aggregates in 3D. 2D angular aggregates were explicitly modelled respectively as ellipses in Song et al. [33], and polygons in Galindo-Torres and Pedroso [34], while ellipsoidal aggregates [35, 36], and polyhedral aggregates [26, 37] were employed in 3D.

### 2.4.2 Random field model

Random field model implicitly assumes different phases of concrete with material properties such as strength and fracture energy as spatially varying random fields. The
random variables are generally controlled by mean and variance value, or even
controlled through definition of covariance functions (see Fig. 2). Therefore, it is very
efficient for generating a large number of samples and becomes convenient for
statistical analysis.

![2D random field](image1.png) ![3D random field](image2.png)

(a) 2D random field (After [38])  (b) 3D random field (After [39])

Fig. 2. Numerical samples characterised by random fields

Many realistic random field models have been developed to represent different
material heterogeneity [40, 41], but limited studies have been carried out for concrete
modelling. Roubin et al. [39] proposed a model based on spatially correlated random
functions to reconstruct meso-structure of concrete. Softening constitutive laws of
concrete were successfully modelled by Weibull random fields in Su et al. [42] for
damage and fracture modelling. Non-uniform stress fields were applied to model size
effect of concrete structures by Vorechovsky [43]. Although being simple and
efficient, this approach can neither explicitly model the inclusions nor consider phase
fraction and their interfaces.

### 2.4.3 Lattice representation

For lattice representation, the material is appropriately subdivided into cells and
lattice sites placed at the cell centres. The deformation of the represented continuum
arises from interactions between the lattice sites. There are, basically, three different
ways to assembly lattices: regular, irregular and mapped assemblies, as shown in Fig.
3 and Fig. 4.

In order to generate a synthetic meso-structure, random distribution of bond
properties according to a given distribution could statistically represent the random
nature of the material in regular and irregular assembled lattice models [8, 44]. The
most straightforward way to include the mechanical properties into the lattice is
simply map a structure on top of the lattice (see Fig. 3(c) and Fig. 4(c)). The material properties of the lattice are defined as mortar or aggregates when both nodes fall inside of the mortar or aggregates. The ITZs are defined when one node falls into the mortar and the other one into aggregates [32].

2.4.4 Image based model

More accurate geometrical models can be generated based on the images from microscope digital cameras [48, 49], however, this technique could only reconstruct 2D sections out of a 3D structure. Recently, X-ray computed tomography (XCT) was developed to overcome this limitation and has been widely used in material science [18, 50-52]. It is a non-destructive 3D imaging technique that uses a series of radiographs to mathematically provide high resolution 3D images of the material (see Fig. 5 and Fig. 6). The images are then converted to meshes for numerical modelling either by using commercial software AVIZO [53] and Simpleware [54], or other self-developed algorithms [18].

XCT becomes popular recently and has been applied by different researchers to study the mechanical behaviour of concrete. Daudeville [55] investigated the role of
coarse aggregates in the triaxial behavior of concrete. Ren et al. [18] studied in situ test of concrete with the system of XCT. Jivkov et al. [8] and Lu et al. [51] employed the XCT to characterize the pore structure in concrete. Wong and Chau [56] investigated the damage mechanisms for normal and high performance concrete. Although several analyses have been successfully performed based on images, it is still noteworthy that conducting XCT experiments is presently very expensive, and generating appropriate meshes from scanned images is time-consuming as coarse mesh may contain distorted elements and fine mesh may reach the limits of computation. Further, the information extracted from analysis of image based models is limited to the imaged microstructure, which may not be statistically representative for larger scale samples or structural components. To achieve representativeness, expensive analysis of a large number of images would be required.

![Tomographic cross-sectional view of three concretes varying by coarse aggregate shape](image1)

**Fig. 5.** Tomographic cross-sectional view of three concretes varying by coarse aggregate shape (After [55])

![Tomographic view of 3D concrete](image2)

**Fig. 6.** Tomographic view of 3D concrete (After [52])

### 2.5 Numerical methodologies

There are many different numerical methods used in the modelling of concrete. The four commonly used methods, e.g. cohesive zone model, damage-plasticity
model, lattice model and SBFEM are reviewed in this thesis. It is worth noting that other numerical methods such as discrete element method (DEM) [20, 57], extended finite element method (XFEM) [58] and boundary element method (BEM) [59] etc. are also proved to be capable for modelling concrete structures.

2.5.1 Cohesive zone model

Cohesive zone modelling has received increasing attention to model crack initiation and propagation. It is an efficient and powerful numerical tool that could be easily implemented in modelling concrete structures. The cohesive zone model was developed by Barenblatt [60, 61] and Dugdale [62], and later extended by Hillerborg et al. [63] for concrete by proposing that de-cohesion can develop anywhere in a structure. This enables the simulation of the energy dissipation in the fracture process zone (FPZ) during crack advance. Park [64] first introduced four stages of the non-linear fracture process of the cohesive zone model, namely stage one representing material without damage, stage two with initiation of micro-cracks, stage three describing the material softening with damage evolution, and stage four defining failure with new cracking surfaces. Recently, cohesive zone modelling has been actively implemented in the modelling of heterogeneous concrete. Lopez et al. [24] and Caballero et al. [26] developed a numerical model using zero-thickness CIEs equipped with fracture-based constitutive law to analyze concrete specimens in 2D and 3D, respectively.

In the cohesive zone model, it is assumed that there exists a normal traction and a tangential traction (shear cohesion) across the crack surfaces, through mechanisms such as material bonding, inclusion interlocking and surface friction in the FPZ. A typical bilinear cohesive zone model for predicting discrete crack propagation in concrete specimens is shown in Fig. 7. A linear ascending branch is added in the softening curve to model the initially un-cracked material. Different CIEs with different constitutive relations need to be specified in the model to represent the potential cracks. The evolution of damage is described via a scalar index $D$ which evolves monotonically from 0 to 1 upon further loading after the initiation of damage as follows,

$$D = \frac{\delta_{mf}(\delta_{m,max} - \delta_{m0})}{\delta_{m,max}(\delta_{mf} - \delta_{m0})}$$

(1)
where $\delta_{m,\text{max}}$ is the maximum effective relative displacement obtained during the loading history, $\delta_{m0}$ and $\delta_{mf}$ denote the effective relative displacements at damage initiation and final failure, respectively.

Damage is assumed to initiate when the following condition is met,

$$\left\{\frac{t_n}{t_{n0}}\right\}^2 + \left\{\frac{t_s}{t_{s0}}\right\}^2 + \left\{\frac{t_t}{t_{t0}}\right\}^2 = 1$$

(2)

The damage initiation and evolution will degrade the unloading and reloading stiffness coefficients $k_n$ and $k_s$, which can be calculated as

$$k_n = (1 - D)k_{n0}, \quad k_s = (1 - D)k_{s0}, \quad k_t = (1 - D)k_{t0}$$

(3)

This affects the tractions, which change according to

$$t_n = \begin{cases} (1 - D)t_n, & t_n \geq 0 \\ t_n, & t_n < 0 \end{cases}$$

(4)

$$t_s = (1 - D)t_s$$

(5)

$$t_t = (1 - D)t_t$$

where $\tilde{t}_n$ and $\tilde{t}_s$ are the traction components predicted by the elastic traction-displacement behaviour for the current separation without damage.

---

Fig. 7. Traction-separation relations for cohesive interface elements

In spite of the potential and promises of the cohesive zone model, a few challenges need to be overcome for a wider application. One of the key issues for a reliable cohesive zone modelling is to have proper material properties where experimental data are usually not available. The interaction between progressive
damage with friction in mixed-mode problems can significantly influence the overall energy dissipation, which might lead to penetration of the cohesive elements and instability in the simulation results.

2.5.2 Damage-plasticity model

Damage-plasticity model has been used successfully in modelling behaviour of concrete and the results showed very good correlations with the experimental data [1, 7, 65, 66]. It is a continuum, plasticity-based damage model, and assumes the main two failure mechanisms are tensile cracking and compressive crushing. This model addresses the degradation of the material stiffness and irreversible deformations since both contribute to the nonlinear response.

Many combinations of damage and plasticity models are widely used for modelling both tensile and compressive failure. Grassl and Jirasek [67] proposed a plastic model with non-local isotropic damage and applied the framework to model concrete under tension and compression. A plasticity and anisotropic damage model was developed for modelling plain concrete using the user subroutine UMAT in ABAQUS [66]. Recently, Kim et al. [7] applied a coupled plasticity-damage model to study the plastic-damage response of concrete meso-structure. Although, damage-plasticity models are widely adopted by researchers, very limited application has been found in modelling meso-structural response of 3D concrete.

Fig. 8 shows a typical uniaxial tensile and compressive response in the damage-plasticity constitutive relation, where the strain in tension and compression can be represented as follows:

\[ \varepsilon_t = \varepsilon_{t}^{ck} + \varepsilon_{t}^{el}, \varepsilon_c = \varepsilon_{c}^{in} + \varepsilon_{c}^{el} \]  \hspace{1cm} (6)

It is assumed in damage-plasticity model that the uniaxial stress-strain curves can be converted into stress versus plastic strain curves using the following equations.

\[ \varepsilon_{t}^{pl} = \varepsilon_{t}^{ck} + \varepsilon_{t}^{el} - \varepsilon_{t}^{in} \]  \hspace{1cm} (7)
\[ \varepsilon_{c}^{pl} = \varepsilon_{c}^{in} + \varepsilon_{c}^{el} - \varepsilon_{c}^{ck} \]  \hspace{1cm} (8)

where \( \varepsilon_{t}^{pl} \) and \( \varepsilon_{c}^{pl} \) are equivalent plastic strain in tension and compression. \( \varepsilon_{t}^{ck} \) and \( \varepsilon_{c}^{in} \) are cracking strain and inelastic strain. \( \varepsilon_{t}^{el}, \varepsilon_{c}^{el}, \varepsilon_{t}^{ck} \) and \( \varepsilon_{c}^{in} \) are calculated as follows:

\[ \varepsilon_{t}^{el} = \frac{\sigma_t}{E_t}, \varepsilon_{c}^{el} = \frac{\sigma_c}{E_c} \]  \hspace{1cm} (9)
2.5 Numerical methodologies

\[ \varepsilon_i^{el} = \frac{\sigma_i}{(1-d_i)E_o}, \varepsilon_c^{el} = \frac{\sigma_c}{(1-d_c)E_o} \]  

(10)

where \(d_i\) and \(d_c\) are damage variables in tension and compression, respectively.

The stress-strain relations (\(\sigma-\varepsilon\)) under uniaxial tension and compression loading are shown respectively as follows.

\[ \sigma_i = (1-d_i)E_o(\varepsilon_i - \varepsilon_i^{pl}) \]  

(11)

\[ \sigma_c = (1-d_c)E_o(\varepsilon_c - \varepsilon_c^{pl}) \]  

(12)

Substituting Equations (7) and (8) into Equation (9) and using Equations (11) and (12) results in two damage variable for tension and compression, respectively.

\[ d_i = 1 - \frac{\sigma_i/E_o}{\varepsilon_i^{pl}(1/b_i - 1) + \sigma_i/E_o} \]  

(13)

\[ d_c = 1 - \frac{\sigma_c/E_o}{\varepsilon_c^{pl}(1/b_c - 1) + \sigma_c/E_o} \]  

(14)

where \(b_i\) and \(b_c\) are constant factors calibrated with experimental tests, and calculated as \(b_i = \varepsilon_i^{pl}/\varepsilon_i^{ck}\), \(b_c = \varepsilon_c^{pl}/\varepsilon_c^{in}\).

Fig. 8. Uniaxial stress-strain curve with damage

2.5.3 Lattice model

In Lattice models, a material continuum is discritized by using a network of either one-dimensional (1D) spring, truss or beam elements. Connecting bonds can break due to overextension, removing the ability to transfer forces between particles. Failure
of a bond results in the redistribution of the load, which provides a representation of micro-crack interaction and accumulation of damage in quasi-brittle materials like concrete, with the local heterogeneity represented by the failure properties assigned to the discrete elements [68]. It is first proposed by Hrennikoff [69] to replace a material continuum by trusses, and later extended by Schlangen and Van Mier [70] and Karihaloo et al. [71] to the simulation of progressive failure in concrete. The lattice model at the mesoscopic level has been successfully applied to the modelling of micro-cracking, crack branching and bridging in concrete, thus allowing the fracture process to be followed until complete failure [72]. More recently, a bi-regular lattice based on truncated octahedrons which can represent all materials of practical interest has been proposed by Jivkov and Yates [46] and applied to concrete damage evolution modelling [8].

Fracture process is simulated by sequential removal of one lattice beam from the mesh at a time for a typical beam lattice model. The lattice elements are assumed to show linear elastic behaviour and the elements with the highest stress over tensile strength ratio are removed in each step. The failure condition is a combination of the normal force and bending moments [45]:

\[
\frac{\sigma}{f_t} = \frac{N + \alpha \max \left\{ M_i, M_j \right\}}{A W} \geq 1
\]  

where \( f_t \) is the normal force, \( A \) is the cross-sectional area of the lattice element, \( W \) is the sectional modulus of the beams cross section. \( N, M_i \) and \( M_j \) represent the axial force and the bending moments, respectively. The parameter \( \alpha \) describes whether bending plays a more dominant or a restrictive role in this criterion.

There has been an increasing interest in using lattice models for concrete modelling, but one challenging issue associated with this model is the huge demand of computational power.

2.5.4 Scaled boundary finite element method (SBFEM)

A more recent alternative is the SBFEM, which is a semi-analytical method developed by Song and Wolf [73, 74] in the late 1990s. The method combines the advantages of FEM and BEM, with additional advantages: it discretises boundaries only and the spatial dimension is reduced by one like the BEM; no fundamental solutions are required, eliminating singular integrals and expanding the BEM’s applicability considerably [75-78]. It is very efficient in modelling problems with
discontinuities and singularities due to its semi-analytical solutions [79-81]. More recently, several FE-SBFE coupled methods have been developed for crack propagation modelling in quasi-brittle materials [82]. Although these coupled methods offer high accuracy in calculating stress intensity factor (SIFs) by SBFEM and retain flexibility in re-meshing by FEM, it seems still very challenging to extend them to 3D fracture modelling. This is because re-meshing in 3D is extremely complicated, and thus almost all of the relevant publications on fracture propagation by using SBFEM have only been focused in 2D [78, 83-85].

2.6 Size effect

The effect of the meso-structure on the observable response is strong when the specimen size is comparable to the sizes of characteristic constituents. This size dependency of nominal material strength has been known for decades, and has been investigated experimentally and numerically since the early 1990s [86-94]. Various models have been proposed to explain the reason for size effect on material strength. Weibull [95] was probably the first to investigate the size effect and proposed a statistical theory which is known as Weibull’s theory. Later, a multi-fractal scaling law was proposed by Carpinteri [96] and applied to the size effect in failures. Bazant [97] discovered the energetic size effect law for quasi-brittle fracture and verified his law experimentally. However, most of the studies on size effect of concrete are analysed by pre-notched specimens under three-point bending [98-100]. With the stress gradients introduced, such performances are not replications of standard tests or the conditions experienced by the majority of structural components. Therefore, investigations of size effect on specimens without notches under uniaxial loading have become necessary and carried out recently. Gitman et al. [101, 102] analysed the size effect of concrete and investigated the existence of representative volume element (RVE) of concrete at different loading regimes. Although the size effect of specimens without notches has been addressed to date, it appears that most of current numerical studies are still focused on 2D and more comparisons between numerical work and experiments are needed to validate the proposed size effect laws.

2.7 Summary of literature review

As been discussed in the previous sections in this chapter, the main challenges lie in the following aspects: (1) Characterization and representation of heterogeneous
concrete samples at the mesoscale. It should be noted that pores/voids which exist in concrete at mesoscale have been found to have severe adverse effects on the specimen strength. In order to take into account of the pores/voids, a detailed procedure for automatic generation of concrete specimens with both randomly distributed aggregates and pores/voids of different shapes has been developed in this study. A “generate-and-place” procedure to simulate concrete with circular, elliptical and polygonal aggregates in 2D is developed in Chapter 3 [27]. A more efficient three-level hierarchical method to generate concrete with spherical, ellipsoidal, polyhedral aggregates and spherical, ellipsoidal voids are developed in Chapter 5 [103]. (2) Development of numerical methodologies for accurate simulation of concrete. Although a lot of numerical methods have been employed to study the mechanical behaviour of concrete, accurate and efficient prediction of fracture, which are significant for engineering applications, are still rare. Successful implementations in the failure and damage modelling of concrete have been pursued in Chapter 2 to Chapter 6, where the commercial finite element package ABAQUS [104] is used equipped with zero thickness CIEs inserted into every solid element to simulate damage and failure of concrete. The mechanical behaviour of concrete in both tension and compression are investigated by a damage plasticity model with non-zero thickness representation of ITZs in Chapter 7 [28]. Non-matching FE-SBFE coupled method is proposed in Chapter 8 to simulate fracture propagation based on the linear elastic fracture mechanics to obtain high accuracy and reduce the computational cost [105]. (3) Size effect of concrete in standard tests. As most of the studies on size effect of concrete analysed by pre-notched specimens under three-point bending are not replications of standard tests, thus size effect on specimens without notches under uniaxial loading is investigated on both strength and toughness by Monte Carlo simulations of mesoscale specimens of varying sizes in Chapter 4 [106].

2.8 References

References


2.8 References


2.8 References

CHAPTER THREE

Monte Carlo Simulations of Mesoscale Fracture Modelling of Concrete with Random Aggregates and Pores

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3.1 Statement of own contributions in joint authorship

Main research idea development and technological planning;
Preparation of tables and figures, and writing of the manuscript;
In-house APDL, MATLAB and FORTRAN programs development for pre-processing in 2D;
Finite element calculation using ABAQUS;
Python script writing for data processing;
Statistical analysis and result interpretation.

3.2 Paper in the research context

This paper presents a systematic study of statistical effects of key multi-phase parameters on the complex fracture behaviour of concrete specimens. Firstly, the details of the developed heterogonous material generator (HMG) and the proposed intersection and overlap checking algorithms for randomly distributed 2D circular, elliptical, polygonal inclusions and circular, elliptical pores are presented. Secondly, 2D constitutive model for CIEs and Monte Carlo simulations for statistical analysis have also been stated. Concrete as one of the quasi-brittle materials is analyzed at mesoscopic level. The generated geometric models are meshed automatically, solved
by FEM, and statistically analyzed. The results obtained by this computational technology are critically analyzed, leading to valuable statistical results: fracture behaviour and stress-displacement responses of the numerical specimens are highly dependent on the random meso-structures; using polygonal rather than circular/elliptical aggregates, or increasing the aggregate volume fraction/porosity will reduce the tensile strength of specimens.

3.3 Addendum

1. Line 2-3 (right column), Page 37 in the published paper: the aggregate area refers to the area fraction of aggregate, and the volume fraction is used when a unit thickness is taken into account in 2D.

2. Table 2, Page 39 in the published paper: due to the difficulty in measuring the material properties for cohesive zone modelling and the specimen is dominated by tensile behaviour of each meso-phase under pure tension, it is assumed in this study that the tensile and shear strength of the CIEs are the same.

3. Figure 9, Page 39 in the published paper: triangular plane stress elements are used to generate solid FE mesh.

4. Figure 11, Page 40 in the published paper: though there is little difference between the results for the three mesh sizes, more coarse mesh is not used in study due to the constraint in meshing.

5. Figure 12, Page 40 in the published paper: longer loading time is not applied because the current model does not include viscosity (creep/relaxation).

6. Figure 18, Page 42 in the published paper: the material properties used in this paper are the same as used by Lopez et al., while the numerical model adopted by Lopez et al. in Ref. [8] is a plastic interface model based on the use of zero thickness CIEs, where the initial failure is given as a three-parameter (tensile strength, cohesion and friction angle) hyperbola and two different fracture energies are used. The experimental data from Hordijk for normal concrete was also compared with the numerical result by Lopez et al. in Ref. [8], and we suggest that more physical tests of material properties be conducted for quantitative comparison between results obtained by simulations and experiments.

7. Figure 25, Page 44 in the published paper: the results on the effect of aggregate and pore shapes are obtained under the assumption that the strength and fracture energy of the mortar-aggregate interface elements were assumed to be the same for
different aggregate shapes. However, it may not be true for the experimental specimens where the adhesion is expected to be higher for crushed aggregates than that for gravel ones. This factor could also be considered in the numerical modelling by increasing the cohesive strength and energy of the mortar-aggregate interfaces, which is beyond the scope of this study.

This Chapter is an exact copy of the journal paper referred to above.
(See Paper I as follows)
Monte Carlo simulations of mesoscale fracture modelling of concrete with random aggregates and pores

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HIGHLIGHTS

- A procedure is devised to generate mesoscale concrete samples with random multi-phases.
- Complex crack initiation and propagation is realised using cohesive interface elements.
- Samples in tension fail with 1 or 2 cracks, regardless of aggregates' and pores' shape and fraction.
- The effects of aggregate shape and porosity should not be neglected in meso-modelling.

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ABSTRACT

A procedure for generating two-dimensional heterogeneous meso-scale concrete samples is developed, in which the multi-phasic features including the shape, size, volume fraction and spatial distribution of aggregates and pores are randomised. Zero-thickness cohesive interface elements with softening traction–separation relations are pre-inserted within solid element meshes to simulate complex crack initiation and propagation. Extensive Monte Carlo simulations (MCS) of uniaxial tension tests were carried out to investigate the effects of key multi-phasic features on the fracture patterns and load-carrying capacities. It is found that the fracture behaviour and stress-displacement responses of the numerical specimens are highly dependent on the random mesostructures, especially the post-peak softening responses. The specimens fail with either one or two macro-cracks, regardless of the shapes and volume fractions of aggregates and pores. Assuming that the aggregate–mortar interface is weaker than the mortar, using polygonal rather than circular or elliptical aggregates, or increasing the aggregate volume fraction will reduce the tensile strength of specimens. The porosity is found to have severely adverse effects on the specimen strength and cannot be neglected in mesoscale fracture modelling of concrete.

1. Introduction

Concrete is a composite material with multiple phases including mortar, aggregates, interfaces and various defects such as pores and weak inclusions. Its mechanical behaviour is a result of multiple mechanisms occurring at different length scales, from macro, meso to microscale and even atomic or sub-atomic scales. Therefore, multi-scale experiments and simulations of concrete has become a hot research area offering more accurate insights to the mechanical behaviour of concrete material and structures [1–4]. A current focus has been stochastic heterogeneous modelling of concrete considering its multiple phases and interactions at micro and meso scales [5–13]. This is desirable, as such small-scale models take into account accurate internal structures so that more fundamental understanding of damage and failure mechanisms can be gained, and more representative homogenised material properties can be used in higher-scale models [13–16]. As concrete is generally used in large-sized structures, meso-scale rather than micro-scale modelling seems a more feasible choice and will be the topic of this study.

There are basically two approaches to generate meso-scale models of concrete: the digital image based approach and the...
parameterization modelling approach. In the former, cameras, microscopes, or more advanced 3D techniques such as nuclear magnetic resonance spectroscopy and X-ray computed tomography (XCT) scanners are used to capture digital images of the mesostructures; the images are then converted into finite element (FE) meshes modelling multi-phases with real sizes, shapes and distributions [12,17–19]. The image-based models are real reflections of the material mesostructures and thus offer tremendous potential. However, it is still costly and time-consuming to conduct 3D tests, and even more so when a large number of samples are usually needed to make meaningful statistical analyses. In addition, image processing and mesh generation of complicated mesostructures is not a trivial task.

In the parameterization modelling approach, indirect and direct algorithms can be used to generate mesostructures. In the indirect algorithms, different phases of concrete are not explicitly modelled; instead, the heterogeneous material properties are modelled as spatially-varying random fields assigned to conventional FE meshes (e.g. [6,7]), or by lattice elements randomly assigned as aggregates and mortar phases in lattice models (e.g. [19,20]). In the direct algorithms, aggregates of different shapes and sizes are generated, randomly packed into a space, and incorporated with mortar to form digital concrete specimens (e.g. [8–11]). The indirect algorithms are able to generate a large number of samples with ease and thus are very promising for global statistical analyses. The direct algorithms can take into account key multi-phasic parameters such as the shape, size, gradation and spatial distribution of pores and aggregates, phase volume fractions and aggregate-mortar interfaces, and their effects on mechanical behaviour of specimens. This makes the direct algorithms attractive in meso-scale modelling, especially when accurate understanding of detailed failure mechanisms is required.

Recent XCT scanned images [19,21,25] show that a large number of pores exist in concrete at micro and meso scales. The pores may have significant effects on the damage and fracture behaviour of concrete specimens. However, they are rarely considered in existing meso-scale models, in which concrete is treated as either a two-phase (mortar and aggregates) or three-phase (mortar, aggregates and interfaces) material.

This paper presents a systematic study of statistical effects of key multi-phasic parameters on the complex fracture behaviour and load-carrying capacities of concrete specimens, through extensive Monte Carlo simulations (MCS) of direct meso-scale finite element models. A generate-and-place procedure similar to [10] is developed to generate 2D mesostructures with randomly packed aggregates and pores of different shapes and fractions. The mesostructures are then meshed automatically using the pre-processing functionalities in ANSYS. Zero-thickness cohesive interface elements governed by nonlinear normal and shear traction–separation laws are then inserted within aggregate, mortar and their interfaces to simulate complex crack initiation and propagation, using a procedure augmented from that in [6]. Finally, the nonlinear finite element models are solved using ABAQUS. The MCS results are critically analysed, leading to valuable statistical results that may help improve designs of concrete material and structures.

2. Generation of mesostructures and finite element models

2.1. Size distribution of aggregates and pores

The optimal gradation or size distribution of aggregates is often determined by the Fuller curve as [13]

\[ P(d) = 100 \left( \frac{d}{d_{\text{max}}} \right)^n \]  

where \( P(d) \) is the cumulative percentage passing a sieve with aperture diameter \( d \), \( d_{\text{max}} \) is the maximum size of aggregates and \( n \) is a constant (\( n = 0.45–0.70 \)), respectively.

Eq. (1) can be discretised into a number of segments, and the area of aggregates within a grading segment \([d_i, d_{i+1}]\) is [10]

\[ A_{\text{agg}}(d_{i+1} - d_i) = \frac{P(d_{i+1}) - P(d_i)}{P(d_{\text{max}}) - P(d_{\text{min}})} \times P_{\text{agg}} \times A \]

where \( d_{\text{min}} \) is the maximum and minimum sizes of aggregates, \( P_{\text{agg}} \) is the area fraction of all aggregates with respect to the total area of concrete sample \( A \).

The aggregates generally occupy 60–80% in volume of the concrete. The aggregate size distribution in [22] is used in this study. Table 1 lists the sieve size ranges with passing and retaining percentages, with the corresponding four-segment gradation curve shown in Fig. 1. For simplicity, only coarse aggregates larger than 2.36 mm are modelled in this study, while the large number of smaller fine aggregates together with the cement matrix is treated as mortar, whose mechanical properties are assumed to be uniform. For normal strength concrete, coarse aggregates usually represent 40–50% of the concrete volume [13].

For simplicity, it is assumed that the pores are circular or elliptical, with a single size range 2–4 mm. The pore area fraction is specified by the porosity \( P_{\text{pore}} \).

2.2. Aggregate and pore generation

A similar procedure presented by Wang et al. [10] is devised. The basic idea is to generate and place aggregates and pores in a repeated manner, until the target area is fully packed. The aggregate shape depends on its type, namely, circular or elliptical for gravels and polygonal for crushed ones. The detailed procedure is as follows.

<table>
<thead>
<tr>
<th>Sieve size (mm)</th>
<th>Total percentage passing (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>19.00</td>
<td>100</td>
</tr>
<tr>
<td>12.70</td>
<td>97</td>
</tr>
<tr>
<td>9.50</td>
<td>61</td>
</tr>
<tr>
<td>4.75</td>
<td>10</td>
</tr>
<tr>
<td>2.36</td>
<td>1.4</td>
</tr>
</tbody>
</table>

Fig. 1. Aggregate size distribution curve with 4 grading segments.
(1) Input controlling parameters. The key parameters include the aggregate type and shape, the Fuller curve, the aggregate area/volume fraction $P_{agg}$, the pore shape, the porosity $P_{pore}$, the size range of pores ($d_0 = 2$ mm, $d_1 = 4$ mm), the minimum distance of aggregates/pores to the specimen boundary $\gamma_1$, and the minimum distance between aggregates/pores or film thickness $\gamma_2$. The minimum distance $\gamma_2$ reflects that each aggregate is coated all around with a layer of mortar. The aspect ratio ranges for elliptical aggregates ($R_1$) and pores ($R_2$), and the number of sides ($N$) and angle range ($\theta$) for polygonal aggregates, are also specified.

(2) Generate a pore. Assuming a uniform distribution between $d_0$ and $d_1$, the pore size is calculated by $d = d_0 + \eta \times (d_1 - d_0)$ where $\eta$ is a random number between 0 and 1. If the pore is elliptical, a random orientation angle is also generated.

(3) Place the pore. Random numbers are generated to define the position (and orientation if elliptical) of the newly generated pore, and the following conditions are checked: (1) the whole pore must be inside the concrete area and (2) there is no overlapping/intersection between this pore and all the existing ones. For circular pores, the condition (2) can be checked easily by comparing the distance between pore centres and the sum of two radii. For elliptical and polygonal pores, the search algorithm in [23] and the convex hull algorithm in MATLAB are used. When both conditions are satisfied, the pore is placed; or otherwise another set of random numbers are generated to place the pore in a new position.

(4) Generate and place all pores. Steps 2 and 3 are repeated until the area of pore remaining to be generated is less than $\pi d_0/4$, i.e. there is no space to place another pore.

---

**Fig. 2.** Numerical samples with gravel aggregates ($P_{agg} = 45\%$).

- (a) Circular aggregates ($P_{pore}=0\%$)
- (b) Circular aggregates and circular pores ($P_{pore}=2\%$)
- (c) Circular aggregates and elliptical pores ($P_{pore}=2\%$)
- (d) Elliptical aggregates ($P_{pore}=0\%$)
- (e) Elliptical aggregates and circular pores ($P_{pore}=2\%$)
- (f) Elliptical aggregates and elliptical pores ($P_{pore}=2\%$)

**Fig. 3.** Numerical samples with different aggregate fraction ($P_{pore} = 2\%$).

- (a) Elliptical aggregates and elliptical pores ($P_{agg}=40\%$)
- (b) Elliptical aggregates and elliptical pores ($P_{agg}=45\%$)
- (c) Elliptical aggregates and elliptical pores ($P_{agg}=50\%$)
Fig. 4. Numerical samples with different porosity ($P_{agg} = 40\%$). (a) Elliptical aggregates and elliptical pores ($P_{pore} = 1\%$). (b) Elliptical aggregates and elliptical pores ($P_{pore} = 3\%$). (c) Elliptical aggregates and elliptical pores ($P_{pore} = 6\%$).

Fig. 5. Numerical samples with different aggregate aspect ratios ($P_{agg} = 40\%, P_{pore} = 2\%$). (a) $R_1 = [1, 1.5]$. (b) $R_1 = [2, 2.5]$. (c) $R_1 = [3, 3.5]$.

Fig. 6. Numerically samples with crushed aggregates ($P_{agg} = 40\%, P_{pore} = 2\%$). (a) Circular pores. (b) Elliptical pores. (c) An XCT image [21].

Fig. 7. A finite element mesh showing different cohesive interface elements. (a) In aggregates. (b) In mortar. (c) On aggregate–mortar interfaces.
Generate an aggregate. This starts with the grading segment containing the largest aggregates. For different grading segments, assuming a uniform distribution between $d_i$ and $d_{i+1}$, the aggregate size $d$ is calculated by $d = d_i + \eta \times (d_{i+1} - d_i)$ where $\eta$ is a random number between 0 and 1.

Place the aggregate. Random numbers are generated to define the position (and orientation if elliptical) of the aggregate. Four conditions are checked before placement: (1) the whole aggregate must be within the concrete area; (2) there is no overlapping/intersection between this aggregate and any existing pores and aggregates; (3) there is a minimum distance between the edge of an aggregate ($\gamma_1$) and the specimen boundary; and (4) there is a minimum gap between any two aggregates ($\gamma_2$). The last two conditions are checked after the aggregate size is enlarged to $(1 + \gamma_1)$ and $(1 + \gamma_2)$ times its size, respectively. If either condition is violated, this aggregate is disregarded and another set of random numbers are generated to place it in a new position. When all the conditions are satisfied, the aggregate is placed.

Generate and place all aggregates. Steps 5 and 6 are repeated until the remaining area to be generated is less than $\pi d_i^2/4$.

The remaining area is then transferred to the next smaller grading segment. Step 5 to step 7 are repeated for all other size grading segments until the last aggregate of smallest size is generated and placed.

Using the above generation-placing procedure, numerical concrete specimens consisting of various shapes, sizes and distributions of aggregates/pores can be built with ease. All the numerical specimens shown in this paper are 50 mm squares, and the aspect ratio ranges $R_1 = R_2 = \{2, 2.5\}$ and the film thickness $\gamma_1 = \gamma_2 = 0.5$ mm are used when elliptical aggregates and pores exist. For crushed polygonal aggregates, $N = \{3, 7\}$ and $\theta = 15^\circ$, $180^\circ$ are used. The 4-segment aggregate gradation curve in Fig. 1 are used for all the samples.

Fig. 2 shows a few examples of numerical samples with combinations of different shapes of gravel aggregates ($P_{agg} = 45\%$ area fraction) and pores of varying porosity.

Fig. 3 shows numerical samples with the same porosity 2% and aggregate area fraction 40%, 45% and 50%. Numerical samples with the same aggregate area fraction 40% and the porosity 1%, 3% and 6% are shown in Fig. 4. The effect of aspect ratios of elliptical aggregates can be seen in Fig. 5. Some numerical specimens with crushed aggregates are shown in Fig. 6, compared with an XCT image of a real concrete specimen [21].

### Finite element mesh generation and fracture modelling

The pre-processing functionalities of ANSYS are utilized to mesh the numerical samples. As the regions of aggregates and pores are already known, the mortar regions are identified by applying the “overlapping” Boolean operations. The samples are then meshed using solid FE elements. The mesh generation process is automated by running a batch file of APDL programs, so that a large number of samples can be meshed quickly for Monte Carlo simulations and statistical analyses.

To simulate realistic fracture processes, 4-noded cohesive interface elements (CIEs) with zero in-plane thickness are then inserted.
into the generated solid FE mesh. The detailed CIE insertion procedure devised for homogeneous materials in [6] is extended to account for multi-phases and interfaces. Three sets of CIEs with different traction–separation softening laws are inserted, namely, CIE\_AGG inside the aggregates, CIE\_MOR inside the mortar, and CIE\_INT on the aggregate–mortar interfaces. As the aggregates have much higher strength than the cement and the interfaces in normal concrete, no cracks are allowed to initiate inside the aggregates by assuming elastic behaviour without damage in CIE\_AGG. However, it is possible to model crack propagation through aggregates (e.g. in lightweight concrete) by assigning damage properties to CIEs in aggregates.

A final FE mesh (element size = 1 mm) after the insertion of CIEs is shown in Fig. 7. The CIEs are highlighted as red lines. Triangular solid FE elements are used because they are flexible in modelling realistic, smooth crack paths.

3. Monte Carlo simulations

Uniaxial tension tests of 50 mm × 50 mm numerical specimens were modelled in this study (see Fig. 8). All the models were fixed at the left boundary and were subjected to a uniformly distributed displacement at the right boundary, i.e. a displacement-controlled loading scheme was used. All analyses were ended at a displacement $d = 0.1$ mm or strain $\varepsilon = 0.002$.

The solid elements for aggregates and mortar were assumed to behave linear elastically. The linear tension/shear softening laws were used to model CIEs [6] with quadratic nominal stress initiation criterion and linear damage evolution criterion. For comparison of results, the same material properties as in [8] were used in this study. They are listed in Table 2. Due to the lack of experimental data, the shear fracture properties were assumed to be the same as the normal ones.

Extensive Monte Carlo simulations were conducted to investigate the effects of key multi-phasic parameters on the statistical responses of numerical specimens. The reference samples have a combination of elliptical aggregates and elliptical pores with $P_{agg} = 40\%$ and $P_{pore} = 2\%$ (Fig. 7). For each MCS, 100 samples were modelled to ensure that the results were statistically converged.

A typical MSC using the ABAQUS/Explicit solver and a mesh in Fig. 7 took about 10 h by parallel computation using 12 Intel Xeon CPUs @ 2.8 GHz.

3.1. Mesh dependence

The method of pre-inserting CIEs may artificially weaken the sample although a very high elastic stiffness is used for CIEs...
The crack pattern may also be mesh-dependent as only CIEs can become cracks. Therefore, a mesh convergence study was conducted first. Three meshes with element length $L_e = 1$ mm, 0.75 mm and 0.5 mm, respectively were modelled for a particular sample shown in Fig. 9. The mesh 1 has 20,346 nodes, 6782 solid elements and 10,004 cohesive elements. The numbers for the mesh 2 and 3 are 33,288, 11,096 and 16,423, and 71,652, 23,884 and 35,504, respectively. Fig. 10 shows that the final crack paths are very similar with little mesh-dependence. The cracks are represented by red cohesive interface elements with damage index $D > 0.9$ ($D = 1$ means complete failure). A magnification factor 10 was used for all deformed meshes unless specified otherwise.

For each element length, 100 numerical samples with random distribution of elliptical aggregates and pores were then generated and analysed. The mean stress–displacement ($\sigma$–$d$) curves for each element length are compared in Fig. 11. The stress is the total horizontal reaction force of all the left boundary nodes divided by the specimen cross-section area. It is clear that there exists little mesh dependence as the curves are almost coincident. Considering the balance between accuracy and efficiency, the element length 1 mm (mesh 1) was used in all the meshes in the following simulations.

### 3.2. Effects of loading time

When the ABAQUS/Explicit solver is used to model quasi-static loading conditions, the loading/step time must be long enough to...
minimise dynamic effects. However, a long loading time results in high computational cost. Fig. 12 shows the $\sigma$–$d$ curves from 100 random samples for three loading times. It can be seen that 0.001 s loading time results in dynamic oscillations in the curves, while smooth and identical curves are obtained for 0.01 s and 0.1 s. Therefore, a loading time 0.01 s was used in all the following simulations.

3.3. Stress–displacement curves and effect of sample number

Fig. 13 shows the $\sigma$–$d$ curves computed from 100 samples with random distribution of elliptical aggregates and pores. The mean curve, the mean and standard deviation of the peak stress (strength) are also shown. The scatter demonstrates the necessity of Monte Carlo simulations with random distributions of phases. Fig. 14 shows the probability density and the best fit Gaussian probability density function (PDF) of the peak stress, which can be used to calculate structural reliability or failure probability against given external loadings and material properties for structural design [6].

Fig. 15 shows the variation of standard deviation in stress with displacement. Before the peak stress is reached at about $d = 0.01$ mm (see Fig. 13), the standard deviation of the stress is lower than 0.1 MPa. It increases to over 0.5 MPa at $d = 0.02$ mm in the post-peak part and decreases afterwards. So the softening response is more sensitive to pore and aggregate distributions than the peak stress.

Figs. 16 and 17 show the effect of the number of samples on the mean and standard deviation of peak stress, respectively. It is clear that 100 random samples are enough to achieve statistical convergence. This is consistent with the conclusion drawn from an MSC study using the indirect modelling approach based on Weibull random fields [6].

In Fig. 18, the mean $\sigma$–$d$ curve from 100 samples is compared with the results from the experiment by Hordijk [24] and the FE simulation by Lopez et al. [8]. It can be seen that the peak loads and the post-peak softening stages of three curves are close. However, one should not intend to compare the curves directly, as they are responses of specimens with different sizes and different distributions and volume fractions of phases.

3.4. Crack propagation and fracture patterns

Two typical fracture patterns were observed in the 100 samples under uniaxial tension. In all the samples, many microcracks initiate in the early stages of loading on the aggregate–mortar interfaces due to their lower fracture properties than the mortar.
The microcracks at peak loads are shown in Fig. 19(a) and 20(a), respectively. It can be seen that at the peak load, there is still no evident macrocracks. The predicted post-peak macrocrack propagation process is illustrated in Figs. 19(b–c) and 20(b–c), in which the different phases are also shown. As the displacement increases, some aggregate–mortar interfacial cracks continue to propagate and are gradually coalesced with newly formed cracks in the mortar. The specimen fails either with one dominant crack (type I in Fig. 19(c)) or with two (type II in Fig. 20(c)). It should be noted that the microcracks in Figs. 19(a) and 20(a) still exist, but they are not shown in Figs. 19c–d and 20c–d because their width is much smaller than that of the macrocracks. A deformation magnification factor = 50 is used in Figs. 19 and 20 to clearly illustrate the detailed microcrack initiation and propagation process.

Among the 100 numerical samples investigated, 58 samples behave as Type I cracking and 42 as Type II cracking. Fig. 21 shows the \( \sigma-d \) curves separately for both types of cracking. It can be seen that the pre-peak responses are almost identical, and there is little difference in the peak stress. However, the post-peak stress drops more quickly in Type I than Type II, leading to lower dissipated energy in Type I cracking. This behaviour may be attributed to smaller fracture area in the single crack in the former than the two cracks in the latter.

3.5. Effects of aggregate volume fraction and porosity

Fig. 22 shows the mean \( \sigma-d \) curves and corresponding peak stress for four aggregate volume fraction \( \rho_{agg} \) ranging from 20% to 50% with 100 samples each. It can be seen that the initial elastic stiffness of the specimens increases as more aggregates are added, which is expected. It is surprising to see that the computed mean tensile strength decreases. This is because the tensile strength is not determined by the number or strength of aggregates, but by the cohesive strength of CIEs that form the microcracks (see Figs. 19a and 20a). A higher \( \rho_{agg} \) means more aggregates and thus more aggregate–mortar interfacial CIEs in the sample. Therefore, more aggregate–mortar interfacial CIEs and fewer mortar CIEs

![Fig. 21. Stress–displacement curves of different cracking types.](image)

![Fig. 22. Effects of aggregate volume fraction \( (\rho_{agg} = 2\%) \). (a) Mean stress–displacement curve. (b) Peak stress.](image)

![Fig. 23. Effects of porosity \( (\rho_{agg} = 40\%) \). (a) Mean stress–displacement curve. (b) Peak stress.](image)
become microcracks to resist the external loading. Because it is assumed that the cohesive strength of the interfacial CIEs is only half that of the mortar CIEs (Table 2), the specimen strength is reduced as $P_{agg}$ increases. This conclusion only holds if such an assumption is valid.

The effects of porosity on the load-carrying capacity are shown in Fig. 23. A higher porosity results in lower strength, because more pores reduce the effective area to resist the tensile force. An increase of porosity from 0% to 6% reduces the strength by 26% (3.80–2.80 MPa).

### 3.6. Effects of aggregate and pore shapes

Apart from the reference samples using elliptical aggregates and pores, additional five combinations of different shapes of aggregates and pores were investigated, with 100 samples generated and modelled for each combination. Some typical crack patterns are shown in Fig. 24. It can be seen that both types of cracking occur regardless of the shapes of aggregates and pores.

Fig. 25 compares the mean $\sigma$–$d$ curves for the six combinations. It seems that given the same volume fractions of aggregates and pores.

### Table 3

<table>
<thead>
<tr>
<th>Shape</th>
<th>Aggregate–mortar Interface elements</th>
<th>Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Circular aggregates &amp; circular pores</td>
<td>672</td>
<td>/</td>
</tr>
<tr>
<td>Circular aggregates &amp; elliptical pores</td>
<td>688</td>
<td>1.02</td>
</tr>
<tr>
<td>Elliptical aggregates &amp; circular pores</td>
<td>1164</td>
<td>1.73</td>
</tr>
<tr>
<td>Elliptical aggregates &amp; elliptical pores</td>
<td>1222</td>
<td>1.78</td>
</tr>
<tr>
<td>Polygonal aggregates &amp; circular pores</td>
<td>1306</td>
<td>1.94</td>
</tr>
<tr>
<td>Polygonal aggregates &amp; elliptical pores</td>
<td>1366</td>
<td>2.03</td>
</tr>
</tbody>
</table>
pores, the mean peak stress for the samples with circular aggregates (3.59 MPa and 3.55 MPa) or elliptical ones (3.54 MPa and 3.49 MPa) is a little higher than that of polygonal-aggregate samples (3.38 MPa and 3.35 MPa). This may be because the specimens with unsound polygonal aggregates have more aggregate–mortar interface elements (see Table 3) that tend to reduce the tensile strength as the aggregate volume fraction does, as discussed in Section 3.5. It may also be caused by the higher stress concentration at the corners of the polygonal aggregates, while the smooth edges of the circular and elliptical aggregates have a more benign stress distribution which delays the fracture event and increases the tensile strength.

4. Conclusions
Numerical models of concrete with random mesostructures comprising circular, elliptical, or polygonal aggregates and circular or elliptical pores have been developed in this study. The complex mesoscale crack initiation and propagation was realistically simulated using the technique of pre-embedding cohesive interface elements. Extensive Monte Carlo simulations of uniaxial tension were carried out to investigate the statistical effects of shapes, volume fractions and random distributions of aggregates and pores. The main conclusions are:

(1) The fracture behaviour and stress-displacement responses of the numerical specimens are highly dependent on the random mesostructures. The computed pre-peak responses and the peak stress (strength) are insensitive to the distribution of aggregates and pores, but the post-peak softening responses are much more sensitive. Therefore, Monte Carlo simulations of a sufficient number of samples should be simulated for accurate understanding of the post-peak responses;

(2) two cracking types were noticed in the Monte Carlo simulations of 50 mm square specimens under the assumed uniaxial tensile boundary conditions, regardless of the shapes and volume fractions of aggregates and pores, namely, Type I with one dominant macrocrack and Type II with two. The latter shows more progressive post-peak softening responses than the former;

(3) assuming that the aggregate–mortar interface strength is lower than the mortar strength, using polygonal rather than circular or elliptical aggregates, or increasing the aggregate volume fraction will reduce the tensile strength of specimens; and

(4) the porosity has severely adverse effects on the specimen strength, and the pores cannot be neglected in mesoscale fracture modelling of concrete.

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References

Monte Carlo Simulations of Mesoscale Fracture of Concrete with Random Aggregates and Pores: A Size Effect Study

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4.1 Statement of own contributions in joint authorship

Main research idea development and technological planning;
Preparation of tables and figures, and writing of the manuscript;
In-house MATLAB program development for automatic FE modelling;
Data processing and statistical analysis;
Interpretation of results.

4.2 Paper in the research context

This paper presents statistical studies of the size effect under tensile loading in mesoscale concrete with prescribed volume fractions, shapes, size and spatial distributions of aggregates and pores. A series of 2D square numerical concrete specimens with different sizes (without notches) are generated at mesoscopic level by the developed in-house software HMG. The numerical work is performed using the cohesive zone model with zero-thickness CIEs developed in Chapter 3. The statistical aspect is based on the Monte Carlo simulation method proposed in Chapter 3, which is a general and robust tool for processing and estimating the uncertainty/reliability of structural performance. The main results of size effect in concrete with different prescribed parameters are discussed in detail. It is found that the numerical results closely follow Weibull’s stochastic size effect law; both the size effect equations of strength and size relations for different porosities, aggregate volume fractions, are given by curve-fitting the Monte Carlo simulation results.
4.3 Addendum

1. Table 1, Page 263 in the published paper: a different aggregate size distribution (smaller maximum aggregate size) from that in Chapter 2 is used to accommodate the size effect study when very small concrete samples are investigated.

2. Figure 9, Page 268 in the published paper: The ratio between the specimen size and maximum aggregate size is about 1 to 5 for specimen size between 12.5mm and 62.5mm, the ratio might be too low for small size specimens and the analyses presented may be below transition scale. Therefore, more meso-structural specimens are needed and statistical analysis is conducted.

3. Line 5 (Left column) in Page 269, Line 3 (Left column) and Figure 16 in Page 270, and Figure 21 in Page 271 in the published paper: Eq. (2) should be Eq. (9).

This Chapter is an exact copy of the journal paper referred to above.
(See Paper II as follows)
Monte Carlo simulations of mesoscale fracture of concrete with random aggregates and pores: a size effect study

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\section*{Highlights}

- Size effect of concrete studied by realistic mesoscale models and Monte Carlo simulations.
- Key meso-control parameters (aggregate fraction and porosity) considered.
- Weibull size effect laws of strength obtained considering the key parameters.
- Equations relating strength and the key parameters obtained.
- Both aggregate fraction and porosity play significant role.

\section*{Abstract}

Size effect in concrete under tension is studied by Monte Carlo simulations of mesoscale finite element models containing random inclusions (aggregates and pores) with prescribed volume fractions, shapes and size distributions (called meso-structure controls). For a given size and a set of controls, a number of realisations with different spatial distribution of inclusions are simulated to produce statistical data for macroscopic load/stress–strain curves. The complex meso-crack initiation and propagation is captured by pre-inserted cohesive interface elements. The effects of specimen size and meso-structure controls on macroscopic strength and toughness are analysed, and empirical size-effect laws for their dependences are proposed by data regression. It is also shown that the mesoscale porosity affects both strength and toughness and should not be ignored in size effect studies of concrete.

\section*{1. Introduction}

Concrete is a composite material with random arrangements of mesoscale (mm) constituents of different mechanical properties. The effect of the resultant heterogeneous meso-structure on the mechanical behaviour is strong when the specimen size is comparable to the sizes of characteristic constituents, making homogenisation questionable. The effect weakens and the homogenisation becomes increasingly valid as the specimen size increases. This is a "structure–property" explanation of the measurable changes in mechanical behaviour with specimen size, known as the size effect \cite{1,2}. The size effect of concrete has been widely investigated experimentally and numerically since 1990s \cite{1,3–10}. It has been shown that the nominal strength of concrete can decrease significantly with increasing specimen size, which is now regarded as an inherent concrete behaviour \cite{11–13}.

Different theories have been developed to explain the size effect, amongst which the best known are the works of Weibull \cite{14}, Bazant \cite{15} and Carpinteri \cite{16}. It appears that the size effect needs to be investigated by a bottom-up approach, with explicit account of concrete non-homogeneous structure, replicated in specimens of increasing sizes. This is an experimentally challenging task, but can be tackled by increasingly realistic numerical models. For example, Van Mier et al. \cite{1,17} and Grassl et al. \cite{18,19} used discrete lattice model to study the size effect of quasi-brittle materials. Karihaloo et al. \cite{20} and Duan et al. \cite{6} used the fictitious crack model to investigate the size effect on concrete. However, mesoscale numerical studies of the size effect of concrete with statistical analyses are still challenging \cite{21–23}, mainly due to the complex multi-phase composition, the complicated nonlinear multi-cracking behaviour, and substantial computational cost from repetitive simulations.
In this paper, we study the size effect in concrete under tension by Monte Carlo simulations (MCS) of mesoscale specimens of varying sizes. The direct parameterisation modelling technique [24–26] is used to build mesoscale concrete models with randomly-distributed aggregates and pores generated according to prescribed size distributions, shapes and volume fractions. The four different phases, i.e., mortar, aggregates, interfaces and pores are explicitly modelled, allowing for examination of their relative influences on meso/macro mechanical responses. The complex meso-crack initiation, propagation and coalescence into macro-cracks is captured by pre-inserted cohesive interface elements into solid finite element (FE) meshes [23,27]. The detailed procedure and initial results have been presented in [23].

The size effect of concrete nominal strength is mostly analysed by pre-notched beams under three-point bending [20,28–30]. However, such loading conditions complicate the analysis and understanding of the size effect on the failure processes due to the strain and stress gradients introduced. Therefore, this study is focused on analyses of specimens without notches under displacement-controlled uniaxial tension. Such analyses replicate standard tensile tests, where stress concentrator is not present initially. This allows us to study a spatially-distributed micro-cracking prior to localisation into a macroscopic crack, rather than to predefine localisation with the presence of a concentrator. The size effect caused by stochasticity, namely more defects are included as the size increases, and the deterministic size effect caused by nonlinear fracture process, were both taken into account. The macroscopic properties of interest in this study are size and toughness. These are calculated by statistical analyses of a number of realisations. The effects of specimen size and the main meso-structure controls (volume fractions and size distributions of aggregates and pores) on these properties are analysed and empirical expressions for their dependences are proposed.

The outline of the paper is as follows. In Section 2 we present the techniques for generation of inhomogeneous meso-structures and the basics of finite element modelling with cohesive interfacial elements. In Section 3 we report and discuss the results of size effects in concrete with different prescribed parameters and propose several size effect laws based on them. The main conclusions are drawn in Section 4.

2. Model and method

The detailed procedure of generating numerical concrete samples and inserting cohesive interface elements into solid FE meshes has been given in [23] and [27]. Herein only an outline is presented for the convenience of discussion.

2.1. Generation of numerical concrete samples

The size distribution of aggregates in concrete is often described by the Fuller curve [31], which is discretised into a number of segments. The aggregate size distribution reported by Hirsch [32] and summarised in Table 1 is used in this study. The concrete contains coarse and fine aggregates and the cut-off size between coarse and fine aggregates is taken to be 2.36 mm. Here only coarse aggregates are explicitly modelled as meso-scale features. The large number of fine aggregates together with the cement matrix is regarded as mortar with homogenised uniform mechanical properties. The coarse aggregates are considered to have elliptical shape. In most concretes, the volume density of coarse aggregates is between 40% and 50% [33]. Elliptical pores are introduced with uniformly distributed sizes in the range from 2 to 4 mm. The prescribed volume fractions of aggregates and pores (i.e., porosity) are met by generating spatially-distributed random aggregates and pores in a repeated manner until a target area is filled [23].

2D square numerical samples are generated. Fig. 1 shows five typical models with different sizes or length L and Fig. 2 shows five samples with L = 50 mm, using the following parameters: aggregate volume fraction \( P_{agg} = 40\% \), porosity \( P_{pore} = 2\% \), aspect ratio for elliptical aggregates and pores \( R_1 = R_2 = 2, 2.5 \), minimum space between the edge of an aggregate and the specimen boundary \( \gamma_1 = 0.5 \) mm and minimum gap between any two aggregates/ pores \( \gamma_2 = 0.5 \) mm.

### Table 1: Aggregate size distribution [32].

<table>
<thead>
<tr>
<th>Sieve size (mm)</th>
<th>Total percentage retained (%)</th>
<th>Total percentage passing (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>12.70</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>9.50</td>
<td>39</td>
<td>61</td>
</tr>
<tr>
<td>4.75</td>
<td>90</td>
<td>10</td>
</tr>
<tr>
<td>2.36</td>
<td>98.6</td>
<td>1.4</td>
</tr>
</tbody>
</table>

2.2. Finite element mesh generation and fracture modelling

The numerical concrete models are then meshed in ANSYS automatically by running a batch file of APDL programs, so that a large number of samples can be meshed quickly for Monte Carlo simulations and statistical analyses. The 4-noded cohesive interface elements (CIEs) with zero in-plane thickness are then inserted into the generated solid FE mesh (triangular plane stress elements) by an augmented procedure devised for homogeneous materials in [27] to account for multi-phases and interfaces. CIEs with different traction–separation softening laws are inserted inside the aggregates, inside the mortar, and on the aggregate-mortar interfaces, respectively, to simulate the complicated nonlinear fracture behaviour [23,34].

The cohesive element COH2D4 with zero in-plane thickness in ABAQUS is used in this model. Its constitutive behaviour is described by a damage initiation criterion and a damage evolution law. A bilinear cohesive zone model, illustrated in Fig. 3, was used in this work.

The damage is assumed to initiate when the following condition is met:

\[
\left\{ \left( \frac{f_{tm}}{P_{tf}} \right)^2 + \left( \frac{f_{ts}}{P_{ts}} \right)^2 \right\} = 1
\]

where \( \{ \) \) is the Macaulay bracket, i.e.,

\[
\langle \delta_n \rangle = \begin{cases} \delta_n, & \delta_n \geq 0 \text{ (tension)} \\ 0, & \delta_n < 0 \text{ (compression)} \end{cases}
\]

The damage evolution is characterised by a scalar parameter, \( D \), representing the overall extension of the crack across the element caused by all physical mechanisms. It is defined in terms of effective relative displacement \( \delta_n \) given by:

\[
\delta_n = \sqrt{\langle \delta_n \rangle^2 + \delta_s^2}
\]

The definition of the damage parameter \( D \) is:

\[
D = \frac{\delta_{mf}}{\delta_{m,\text{max}} - \delta_{mf}} \frac{\delta_{mf} - \delta_{mf}}{\delta_{m,\text{max}} - \delta_{mf}}
\]

where \( \delta_{m,\text{max}} \) is the maximum effective relative displacement attained during the loading history, and \( \delta_{mf} \) and \( \delta_{m,\text{max}} \) are effective relative displacements corresponding to \( \delta_{mf} \) and \( \delta_{m,\text{max}} \) in Fig. 3, respectively. \( D \) evolves monotonically from 0 to 1 upon further loading after the initiation of damage.

The damage initiation and evolution degrades the unloading and reloading stiffness coefficients, \( k_s \) and \( k_c \), calculated by:
\[ \frac{1}{C_0} D \]

The tractions are also affected by damage according to:

\[ \frac{1}{C_0} D \]

\[ \frac{1}{C_0} D \]

\[ \frac{1}{C_0} D \]

where \( t_n \) and \( t_s \) are the traction components predicted by the elastic traction–displacement behaviour for the current separation without damage.

Material properties, such as density, Young’s modulus, Poisson’s ratio, tensile strength and fracture energy, are set for continuum elements of aggregates and mortar, and for the three sets of interface cohesive elements. The material heterogeneity is represented by different phases with corresponding material properties.

2.3. Definition of macroscopic properties and statistical analyses

The size effects on the tensile strength and toughness are investigated in this study. The strength is defined as the mean value of peak stresses (the peak load divided by the cross-sectional area) on the stress–strain curves, obtained from fracture modelling of a number of numerical samples for each size. The toughness is defined as the mean value of energies consumed per unit volume up to failure, i.e., the area under the stress–strain curve up to the ultimate failure from a number of numerical samples for each size, measured in J/m³.

The Monte Carlo simulation results are evaluated statistically. The standard deviation (SD) \( s \) of \( n \) number of results \( x_i \) \( (i = 1, n) \) is defined as:

\[ s^2 = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x})^2 \]

where \( \bar{x} \) the mean of \( x \). The coefficient of variation (CoV = \( s/\bar{x} \)) is also calculated, to represent the fluctuation of measured property relative to its average value.

3. Results and discussion

3.1. FE modelling setups

Uniaxial tension tests of square numerical specimens were modelled in this study (see Fig. 4). The out-of-plane thickness
was unit and plane stress was assumed. All the models were fixed at the left boundary and subjected to a uniformly distributed displacement at the right boundary, i.e., a displacement-controlled loading scheme was used.

The solid elements for aggregates and mortar were assumed to behave linear elastically. The linear tension/shear softening laws were used to model CIEs with quadratic nominal stress initiation criterion and linear damage evolution criterion. Similar material properties as in [24] were used in this study. Young’s modulus was $7 \times 10^4$ MPa for aggregates and $2.5 \times 10^4$ MPa for mortar. Poisson’s ratio of both aggregates and mortar was 0.2. The cohesive elements inside mortar had elastic stiffness $k_n = k_s = 10^6$ MPa/mm, tensile strength $t_n = 6$ MPa and fracture energy $G_f = 0.06$ N/mm. The cohesive elements on aggregate-mortar interfaces had $k_n = k_s = 10^6$ MPa/mm, $t_n = 3$ MPa and $G_f = 0.03$ N/mm. Elastic behaviour without damage was assigned to the cohesive elements inside aggregates so that no cracks were allowed to initiate inside aggregates as they are much stronger than other phases in normal concrete. Due to the lack of experimental data, the shear fracture properties were assumed to be the same as the normal ones.

Extensive Monte Carlo simulations of numerical samples of different sizes ($L = 12.5, 25, 37.5, 50$ and $62.5$ mm, see Fig. 1) with various meso-structure controls were carried out. The reference samples have a combination of elliptical aggregates and elliptical pores with $P_{agg} = 40\%$ and $P_{pore} = 2\%$ (Figs. 1 and 2). For each MCS, 50 samples were modelled to ensure that the results were

---

### Table 2
Average finite element numbers for specimens of five sizes.

<table>
<thead>
<tr>
<th>Size $L$ (mm)</th>
<th>Total number of elements</th>
<th>Number of cohesive elements</th>
</tr>
</thead>
<tbody>
<tr>
<td>A 12.5</td>
<td>1094</td>
<td>634</td>
</tr>
<tr>
<td>B 25</td>
<td>3960</td>
<td>2350</td>
</tr>
<tr>
<td>C 37.5</td>
<td>9111</td>
<td>5357</td>
</tr>
<tr>
<td>D 50</td>
<td>17,147</td>
<td>10,281</td>
</tr>
<tr>
<td>E 62.5</td>
<td>25,891</td>
<td>15,441</td>
</tr>
</tbody>
</table>

---

![Fig. 4. Geometry and boundary conditions of numerical specimens.](image)

![Fig. 5. Typical fracture process in one sample: the red areas represent cohesive elements with damage level over 0.9. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)](image)
Based on our previous study of mesoscale fracture modelling [23], the element length of 1 mm, the loading time of 0.01 s used in the ABAQUS/Explicit solver, and the final displacement of 0.1 mm were used for all sizes of samples considering the balance between accuracy and efficiency. The presented model has been validated previously [23] by comparison of numerical results with available experimental data and with other numerical studies.

Table 2 shows the average finite element numbers of numerical samples of the five sizes. It can be seen that a considerable number of nonlinear cohesive interface elements are inserted to simulate the fracture process, making computation time-consuming. A typical MCS for $L = 50$ mm took about 5 h by parallel computation using 12 Intel Xeon CPUs @ 2.8 GHz.

### 3.2. Results for samples with $L = 50$ mm

The failure evolution simulated for a typical sample with $L = 50$ mm is illustrated in Fig. 5. Fig. 5a–d shows the deformed meso-structure at elastic stage, at peak stress, in softening branch, and prior to sample disintegration, respectively. Displacement magnification factors of 800, 400, 200 and 30 were used, respectively, to illustrate clearly the meso-crack initiation and propagation process. This evolution is typical for all 50 realisations with variations reflected by statistical analysis of peak stress and toughness as follows.

The stress–strain curves of all 50 samples with the mean curve are plotted in Fig. 6a. The effects of the sample number on the mean and the CoV of peak stress can be seen in Fig. 6b and c, respectively. The results show that 50 samples are enough to obtain a convergent mean peak stress with a stable fluctuation below 4%.

The results with respect to the toughness are shown in Fig. 7a–c, respectively. The number of samples (50) is sufficient to reach a converged mean toughness with a stable fluctuation of about 19%.

The mechanical behaviour of concrete is often characterised by a single specimen or a small number of specimens [24,26,35–38]. The results here show that the stress–strain responses vary with different realisations of specimens, especially in the post-peak stage. Therefore the conclusions based on a small number of analyses could be drawn for the elastic stage only, and substantially more realisations are necessary to yield conclusive results for softening behaviour.

The influence of the sample number on the CoV of peak stress and toughness are shown in Fig. 8a and b respectively for samples of all sizes. It can be seen that 50 samples are enough to reach stationary responses for all sizes.
(a) Toughness-strain curves for 50 concrete samples

(b) Effect of the sample number on the mean toughness

(c) Effect of the sample number on the CoV of toughness

Fig. 7. Statistical analysis of toughness from Monte Carlo simulation.

(a) Influence of sample number on the CoV of peak stress

(b) Influence of sample number on the CoV of toughness

Fig. 8. Influence of sample number on the coefficient of variations.
3.3. Size effects of reference samples

Fig. 9 compares the mean stress–strain curves from 50 realisations each for the specimens of 5 sizes with elliptical inclusions ($P_{agg} = 40\%$, $P_{pore} = 2\%$). It is evident that the strength (mean peak stress) decreases monotonically as the size increases. It can also be seen that the slopes of the post-peak softening parts decrease with increasing size, indicating more brittle behaviour of larger specimens. This is consistent with experimental observations [9,13].

Table 3 summaries the mean, standard deviation and coefficient of variation of the peak stress and the toughness. The same data are also shown in Fig. 10. As the CoV of peak stress decreases when sample size increases, the effect of random aggregate and pore distribution on the peak stress decreases.

The results in Fig. 10 were curve-fitted using the least square method according to Weibull’s size effect law \[14\]

$$\ln r = a + b \ln D$$

where $r$ is the mean nominal strength, $D$ the specimen size, and $a$ and $b$ are regression coefficients. $a = 1.52$ and $b = -0.07$ were found with correlation factor $R^2 = 0.94$, indicating a good agreement with the Weibull theory (Fig. 11). The results with the calculated coefficients match well with Weibull size effect law for Weibull modulus $m = 24$. This comparison provides a support for the soundness of the proposed meso-structure modelling and Monte Carlo simulation approach.

The size effect on toughness is shown in Fig. 12. It can be seen that the sample size has significant effects on the toughness. It is three times more for $L = 12.5\, \text{mm}$ than $L = 62.5\, \text{mm}$. It should be noted that the CoV of toughness is relatively high (about 17.5\%) even after sampling 50 different realisations.

3.4. Influence of aggregate volume fraction

Concrete samples with $L = 25, 37.5, 50$ and 62.5 mm containing elliptical aggregates and pores were studied with variable aggregate volume fraction $P_{agg}$. The size $L = 12.5\, \text{mm}$ is too small to generate samples with large aggregates in Fuller curve when a low $P_{agg}$ is assumed and thus not considered. All other meso-structure parameters were the same as aforementioned in Section 3.1. Typical samples with $P_{agg} = 20–50\%$ are shown in Fig. 13.

Fig. 14 shows the size effect on strength for $P_{agg} = 20\%, 30\%, 40\%$ and 50\%, respectively. To derive a functional relation between the strength and the aggregate volume fraction, additional samples of different sizes with pure mortar (2\% pores) were simulated. Fig. 15 shows the relations between the peak stress and the aggregate volume fraction for different sizes. By curve-fitting, it is found that the following quadratic function can well describe the effect of $P_{agg}$ for all the sizes:

$$\sigma_{agg} = c(P_{agg}^2 - 1.17P_{agg} + 1.35)\sigma_0^{agg}$$

\[10\]
where $\sigma_{agg}^0$ is the strength of pure mortar sample, and $c$ is an empirical coefficient ($c = 0.73$ in this study). It should be noted that Eq. (10) was only tested for aggregate volume fraction from 0% to 50% (coarse aggregates).

The size effect laws (Eq. (2)) for $P_{agg} = 20\text{–}50\%$ were computed by the least square regression and shown in Fig. 16. It can be found that the slope decreases as $P_{agg}$ increases, indicating a reduction of size effect for larger aggregate volume fractions. This may be due to the smaller variation in aggregate spatial distribution for higher $P_{agg}$.

The size effect on toughness for different $P_{agg}$ is shown in Fig. 17. For a given size, an increase of the aggregate volume fraction results in a decrease of toughness.

### Table 3

<table>
<thead>
<tr>
<th>Size $L$ (mm)</th>
<th>12.5</th>
<th>25</th>
<th>37.5</th>
<th>50</th>
<th>62.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean peak stress (MPa)</td>
<td>3.845</td>
<td>3.611</td>
<td>3.514</td>
<td>3.461</td>
<td>3.438</td>
</tr>
<tr>
<td>SD (MPa)</td>
<td>0.288</td>
<td>0.189</td>
<td>0.159</td>
<td>0.139</td>
<td>0.129</td>
</tr>
<tr>
<td>CoV (%)</td>
<td>7.490</td>
<td>5.227</td>
<td>4.528</td>
<td>4.021</td>
<td>3.765</td>
</tr>
<tr>
<td>Mean toughness (kJ/m$^3$)</td>
<td>3.331</td>
<td>2.136</td>
<td>1.552</td>
<td>1.322</td>
<td>1.134</td>
</tr>
<tr>
<td>SD (kJ/m$^3$)</td>
<td>0.267</td>
<td>0.286</td>
<td>0.276</td>
<td>0.236</td>
<td>0.202</td>
</tr>
<tr>
<td>CoV (%)</td>
<td>8.031</td>
<td>13.375</td>
<td>17.759</td>
<td>17.848</td>
<td>17.842</td>
</tr>
</tbody>
</table>

The same as in Section 3.1. Fig. 18 shows a few typical samples with $L = 50$ mm.

The size effect on strength for samples with $P_{pore} = 0\text{–}6\%$ is shown in Fig. 19. It can be seen that the strength decreases as the sample size or porosity increases.

A power function, similar to the one for compression strength in cement paste suggested by Powers [39], is proposed here to relate the specimen strength and the porosity:

$$\sigma_{pore} = \sigma_{pore}^0 (1 - P_{pore})^n$$  \hspace{1cm} (11)

where $\sigma_{pore}^0$ is the specimen strength without pores and $n$ is an empirical value. $n = 4$ is found in this study resulting in good agreement.
agreement between Eq. (11) and the numerical results, as shown in Fig. 20 for all the sizes.

The size effect laws obtained according to Eq. (2) for different porosity are shown in Fig. 21. No definitive trend for the porosity influence on the size effect can be observed. The reason may be that the porosities investigated in this paper (0–6%, typical for standard concrete) are relatively small and therefore the spatial arrangement of the pores has a pronounced impact on the concrete non-linear responses. This means that the simulated number of random distributions might be insufficient to obtain a consistent trend for the effect of porosity on the size effect of peak stress. A consistent trend is expected from simulations with higher porosities, e.g., for porous and foamed concrete, but this is beyond the scope of the present paper.

The size effect on toughness for different porosity is plotted in Fig. 22. For a constant specimen size, it can be observed that a porosity increase results in decreased toughness.

---

Fig. 15. Effect of aggregate volume fraction on peak stress for different sizes (Ppore = 2%).

Fig. 16. Size effect on strength for different aggregate volume fraction (Ppore = 2%): lines are the size effect laws (Eq. (2)) and data points are from modelling.

Fig. 17. Size effect on toughness for different aggregate volume fractions.
Fig. 18. Typical samples with different porosity ($L = 50$ mm, $P_{agg} = 40\%$).

Fig. 19. Size effect on strength for samples with different porosity.

Fig. 20. Effect of porosity on peak stress for different sizes ($P_{agg} = 40\%$).

Fig. 21. Size effect on strength for different porosity ($P_{agg} = 40\%$); lines are the size effect laws (Eq. (2)) and data points are from modelling.

\[ y = -0.059x + 1.572 \quad R^2 = 0.98 \]
\[ y = -0.055x + 1.457 \quad R^2 = 0.98 \]
\[ y = -0.090x + 1.524 \quad R^2 = 0.98 \]
\[ y = -0.069x + 1.354 \quad R^2 = 0.99 \]
and ongoing. Further verification of these findings via 3D models is required since the 2D analysis remains limited to planar crack morphologies, patterns and mean stress–strain curves obtained appear realistic, the aggregate volume fraction, the porosity significantly affect both the Monte Carlo simulations results. It is also shown that as the relations between them and the strength, are given by curve-fitting for different porosities and aggregate volume fractions, and the distribution of deterministic size effect. Both the size-effect equations captured by pre-inserted cohesive interface elements. It is found that the complex meso-crack initiation and propagation is successfully measured and characterized for varying porosity. Fig. 22. Size effect on toughness for varying porosity.

4. Conclusions

In this paper, we have investigated the size effect on strength and toughness in concrete specimens under tension, through extensive Monte Carlo simulations of mesoscale finite element models containing randomly-distributed aggregates and pores with prescribed volume fractions, shapes and size distributions. The complex meso-crack initiation and propagation is successfully captured by pre-inserted cohesive interface elements. It is found that the numerical results closely follow Weibull’s stochastic size effect law, although more research is needed to clarify the contribution of deterministic size effect. Both the size-effect equations for different porosities and aggregate volume fractions, and the relations between them and the strength, are given by curve-fitting the Monte Carlo simulations results. It is also shown that as the aggregate volume fraction, the porosity significantly affect both strength and toughness of the specimens and should not be ignored in size effect studies of concrete. Although the crack patterns and mean stress–strain curves obtained appear realistic, the 2D analysis remains limited to planar crack morphologies, and further verification of these findings via 3D models is required and ongoing.

Acknowledgements

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References

5.1 Statement of own contributions in joint authorship

Main research idea development and technological planning;
Preparation of tables and figures, and writing of the manuscript;
In-house APDL, MATLAB and FORTRAN programs development for pre-processing in 3D;
Finite element calculation by ABAQUS;
Python script writing for data processing;
Statistical analysis and result interpretation.

5.2 Paper in the research context

This paper extends the work in Chapter 3 from 2D to 3D. Similarly, the details of the HMG and the proposed intersection and overlap checking algorithms for randomly distributed 3D spherical, ellipsoidal and polyhedral inclusions and voids are proposed first, followed by the introduction of 3D constitutive model for cohesive interface elements and Monte Carlo simulations for statistical analysis. Plain heterogeneous concrete with random aggregates and voids is analyzed and the outcomes are presented comprehensively. The obtained results provide valuable information for improved understanding of damage and failure mechanisms of concrete: the mechanical response and crack propagation in 3D concrete are affected strongly by the meso-structure, i.e. load-carrying capacity decreases with increasing aggregate or...
void content and increasing aggregate roughness; pre-peak response and peak stress are relatively insensitive to the aggregate and void spatial distribution; post-peak softening response is sensitive to the spatial distribution of aggregates and voids; the cohesive properties of concrete constituents affect strongly the macroscopic mechanical response and the cracking patterns, i.e. critical tensile stress of constituents has direct effect on the peak stress, and differences between the strength of the constituents change the patterns of micro-crack coalescence and macro-crack propagation; cohesive energy has little effect on the pre-peak behaviour, but affects strongly the softening behaviour and cracking paths of concrete under tension.

5.3 Addendum

1. Figure 13, Page 23 in the published paper: similar to 2D modelling, though there is little difference between the results for the three mesh sizes, more coarse mesh is not used in study due to the constraint in meshing.

2. Figure 23 in Page 29 and Figure 24 in Page 30 in the published paper: the figures showing models without CIEs in the middle columns of Figure 23 and Figure 24 are obtained by removing the damaged cohesive elements (damage index $D \geq 0.95$).

3. Figure 26, Page 31 in the published paper: more samples may be needed to extract the information of the relationship between void (and/or aggregate) volume fraction and proportion of Type I and Type II cracking modes. It is computationally demanding especially for 3D, and thus is planned to be finished in the future with the algorithmic and hardware development.

4. Section 4.4, Page 34 in the published paper: the experimental data of critical tensile stress and cohesive energy of the cohesive interfaces are usually not available, and these two parameters may be related while they are assumed to be independent material properties in this study for parametric study.

5. Section 4.4 in Page 34 in the published paper: the critical tensile stress stated refers to the tensile strength of cohesive interfaces.

This Chapter is an exact copy of the journal paper referred to above.
(See Paper III as follows)
Computational technology for analysis of 3D meso-structure effects on damage and failure of concrete

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Abstract: Methodology for analysis of meso-structure effects on longer-scale mechanical response of concrete is developed. Efficient algorithms for particle generation and packing are proposed to represent 3D meso-structures as collections of discrete features distributed randomly in a continuous phase. Specialised to concrete, the continuous phase represents mortar, while the features are aggregates and voids. Intra- and inter-phase cohesive zones are used for failure initiation and crack propagation. A Monte Carlo approach is proposed to analyse the effects of meso-structure geometrical (volume density, size distribution and shape of features) and physical (strength and energy of cohesive zones) properties, whereas a number of model realisations with identical properties are used for statistical analysis. The results present the relative significance of each meso-structure parameter for the emergent load carrying capacity (tensile strength), damage evolution via micro-crack coalescence and macro-crack patterns, and failure energy density (toughness) of concrete. The proposed methodology is an effective tool for meso-structure optimisation in the design of concrete structures with prescribed requirements for strength and toughness.

Keywords: Concrete, Random packing, Voids, 3D, Monte Carlo simulation, Cohesive zone model, Mesoscale modelling

1 Introduction

In structural design, concrete is considered as a homogeneous continuum. This first approximation is acceptable as long as components remain in the elastic regime of deformation, i.e. no energy dissipation mechanisms such as plasticity and surface

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separations (micro-cracking) are activated. When energy dissipation is present, it is
localised, guided and governed by sub-continuum structures, the knowledge of which
is critical for understanding and explaining inelastic and failure behaviour [1].

Concrete is a complex composite with sub-continuum structures at multiple
length scales. The largest length-scale with observable heterogeneity is traditionally
called the meso-scale. Meso-structure of concrete contains voids, aggregates, mortar,
and interfaces between them. As closest to the component scale, the meso-structure
plays a critical role in the observable macroscopic behaviour of concrete [2, 3]. In the
past few decades, a number of meso-scale models considering both meso-structure
and local failure mechanisms have been proposed and developed to understand and
quantify their effects on longer-scale response of concrete.

With respect to the meso-structure representation of concrete, the two main
approaches are the image-based modelling and the parameterization modelling.
Although the meso-structure obtained from images, e.g. using computed tomography,
is closest to nature, it is presently very expensive and time-consuming to generate
sufficient scanned images from samples to make meaningful statistical analyses (e.g.
[4-10]), especially for three-dimensional (3D) problems. For parameterization
modelling, both direct (e.g. [11-15]) and indirect approaches (e.g. [16-22]) have been
widely used to characterize heterogeneous materials. An advantage of the direct
approach is that it allows for varying independent key meso-structure parameters,
such as volume fractions, shape, size and spatial distribution of pores/voids and
aggregates. Because of this feature, the direct approach is particularly suitable for
statistical analysis of damage and failure of concrete performed in this study.

For meso-structure models of concrete, identification and generation of unit cell
geometry is a vital step, since both shape and size of aggregates have significant
influences on stress distribution, crack initiation and damage accumulation up to
macroscopic failure within concrete [23, 24]. Regarding two-dimensional (2D) cases,
particles with regular shapes such as circle, ellipse and polygon are generally used.
Beddow and Meloy [25] proposed a morphological law to acquire rounded aggregates.
Angular aggregates were generated respectively as polygons with prescribed
elongation ratios [26] and convex polygons using Voronoi tessellation method [27].
More recently, Wang et al. [13, 14] developed a “generate-and-place” procedure to
simulate circular, elliptical and polygonal aggregates for meso-scale modelling of
fracture and damage of concrete in 2D.
Regarding 3D cases, aggregates are usually assumed to be spherical for simplicity, as presented in Bazant et al. [28], Man et al. [29] and Wriggers et al. [23]. In recent years, considerable attention has been paid to generating various aggregate shapes, e.g., ellipsoidal aggregates using functions with varying parameters [30-32], and polyhedral aggregates by random packing systems [33, 34] and Voronoi tessellation methods [3, 35, 36]. It is worth noting that most of the existing meso-structure models of concrete only consider random aggregates [3, 11, 12, 37] but neglect voids. However, X-ray computed tomography (XCT) images of concrete [5, 38-41] clearly show that voids exist in concrete at mesoscale. It is therefore imperative to develop a procedure for automatic generation of morphological details of materials with both randomly distributed aggregates and voids of different shapes.

With respect to the numerical models for local material failure (new surface generation, micro-cracking), a number of models have been used to study damage and failure of concrete. The dominant approach at present employs continuum finite element modelling of the constituents with allowance for failure via cohesive interfaces between the continuum solid elements [42-46]. The key element is the behaviour of the cohesive interfaces, based on cohesive zone model developed by Barenblatt [47, 48] and Dugdale [49] and later extended by Hillberbog et al. [50]. For cohesive zone model, the cohesive interface elements (CIEs) are pre-inserted or dynamically inserted into the initial finite element mesh so that realistic crack patterns can be simulated [51]. Because of its simple formation, easy implementation in the form of CIEs, cohesive zone model becomes more and more popular in modelling crack propagation in concrete and other quasi-brittle materials. It should be noted that other numerical methods, such as continuum strong discontinuity approach (CSDA) [52, 53], extended finite element method (XFEM) [54], and embedded finite element method (EFEM) [4] etc. have been used for modelling concrete structures and show growing popularity in dealing with strong discontinuities. Other alternative approaches, such as discrete element models [55] and lattice models [19, 20, 56], have also been developed. A key issue associated with the class of discrete models is the difficulty in determining the model parameters which provide observed macroscopic behaviour, particularly for non-regular arrangements [57]. This is avoided in the continuum-based modelling on the expense of the need to calibrate cohesive laws. Therefore, cohesive zone model is used in this work to represent failure initiation and propagation in concrete.
The aim of this work is to develop a holistic procedure for analysis of mesostructure and local properties effects on the macroscopic behaviour of concrete. The procedure contains three parts: generation of realistic meso-structures, which extends the work of Wang et al. [13] from 2D to 3D; incorporation of cohesive interfaces and description of their properties; Monte Carlo simulations (MCS) with spatially randomised meso-structures and statistical analysis of emergent behaviour of concrete.

Firstly, an in-house program heterogeneous material generator (HMG) consisting of particle generation and packing is developed and applied to generate 3D meso-structures of concrete with randomly distributed spherical, ellipsoidal and polyhedral aggregates and voids, respectively. Secondly, interfaces between all aggregate-aggregate, mortar-mortar and aggregate-mortar continuum elements are represented by zero-thickness cohesive elements via an in-house program cohesive interface elements insertion (CIEIN). Non-linear cohesive laws for the three types of interfaces are implemented. Thirdly, MCS are carried out to investigate the effects of main parameters, such as, shape, size, spatial distribution and volume fractions of aggregate and void, and cohesive laws, on mechanical behaviour of concrete in a quantitative manner. The outcomes are presented comprehensively and provide valuable information for improved understanding of damage and failure mechanisms of concrete. The proposed methodology allows for informed design of concrete structures.

2 Meso-structures of concrete

In this section, details of the developed HMG and the proposed intersection and overlap checking algorithms for random distribution of spherical, ellipsoidal and polyhedral aggregates and voids are presented. The proposed algorithms are suitable for generating a variety of heterogeneous materials, such as cement composites, nuclear graphite, graphene nano-composites, etc. Plain concrete with random aggregates and voids is set as an example in this section.

2.1 Particle size distribution-aggregate and void

The aggregate size distribution of concrete is often characterised by the Fuller curve that represents the gradation of aggregate particles resulting in optimum density and strength of concrete mixture. Fuller curve can be described by [23]
\[ P(d) = 100 \left( \frac{d}{d_{\text{max}}} \right)^n \] (1)

where \( P(d) \) is the cumulative percentage passing a sieve with aperture diameter \( d \), \( d_{\text{max}} \) is the maximum size of aggregate particles, and \( n \) is the exponent of the equation (\( n = 0.45-0.70 \)).

For the ease of numerical implementation, the gradation curve expressed in Equation (1) can be replaced with a number of segments, where the amount of aggregate \( V_{\text{agg}} \) within each grading segment \([d_i, d_{i+1}]\) can be expressed as [26]

\[ V_{\text{agg}}[d_{i+1} - d_i] = \frac{P(d_{i+1}) - P(d_i)}{P(d_{\text{max}}) - P(d_{\text{min}})} \times P_{\text{agg}} \times V \] (2)

where \( d_{\text{max}} \) and \( d_{\text{min}} \) denote the maximum and minimum sizes of aggregates, respectively, \( P_{\text{agg}} \) is the volume fraction of aggregate and \( V \) is the sample volume of concrete.

A typical particle size distribution of coarse aggregates in concrete [58] as given in Table 1 is used in this study. According to their size, aggregates in concrete are generally classified into two categories: fine aggregate (e.g., sand) and coarse aggregate (e.g., gravel and crushed stone). Only coarse aggregates larger than 2.36 mm are considered in this study, while the large number of fine aggregates together with cement matrix is regarded as mortar [59], which keeps the model fidelity and avoids the computational difficulty caused by enormous number of elements. For normal strength concrete cast with a mould in the laboratory, the coarse aggregates typically occupy 30-50% of the concrete volume.

Table 1. Particle size distribution of coarse aggregates in concrete [58]

<table>
<thead>
<tr>
<th>Sieve size (mm)</th>
<th>Total percentage retained (%)</th>
<th>Total percentage passing (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>12.70</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>9.50</td>
<td>39</td>
<td>61</td>
</tr>
<tr>
<td>4.75</td>
<td>90</td>
<td>10</td>
</tr>
<tr>
<td>2.36</td>
<td>98.6</td>
<td>1.4</td>
</tr>
</tbody>
</table>

Mechanical behaviour of concrete is highly related to aggregate, in particular, the shape of the aggregate particles that depends on aggregate type. From X-ray CT
images, it was found that gravel aggregates have a spherical or ellipsoidal shape, while crushed aggregates have a polyhedral shape [41]. It was also observed from CT images that concrete contains a number of voids, especially for rolled and crushed aggregate concrete.

Pores in concrete can be roughly divided into air voids, capillary pores and gel pores. The capillary and gel pores (nanometre or micrometre scales) are too small and outside the scope of mesoscale modelling. Larger pores of dimensions of up to a few millimetres are the result of the air entrapped during mixing and not removed by vibration of fresh concrete [60], which could be clearly observed from CT images at meso-scale [39, 61]. Therefore, it is necessary to include voids in the meso-structure of concrete. In this study, voids with size ranging from 2 to 4 mm as presented in [62] are taken into account. The shape of voids is assumed to be sphere and ellipsoid. The algorithms and procedures to generate individual particle with various shape of sphere, ellipsoid and polyhedron are given in Appendix.

2.2 Particle packing-aggregate and void

Wang et al. [26] presented a comprehensive procedure using a commonly adopted “taking” and “placing” method to generate a 2D random geometric arrangement of aggregates. A similar procedure was adopted in our previous published work for generating 2D meso-structures of concrete with different shape of aggregates and voids [13]. The present study extends it to randomly distribute 3D particles of aggregate and void with various shape into a cube according to the prescribed particle size distribution and density. The flowchart of particle packing composed of “input”, “taking” and “placing” processes is shown in detail in Fig. 1.

The central idea is to create aggregates and voids in the cubic concrete in a repeated manner, until the target volume of aggregates and voids is achieved. The “input” process reads the controlling parameters for generating a meso-structure with random aggregates and voids. The “taking” process generates an individual aggregate or void in accordance with the random size and shape descriptions. The “placing” process subsequently places the aggregates and voids into the predefined area in a random manner, subjected to the prescribed physical constraints. The generation of synthetic 3D meso-structures is implemented in MATLAB [63].
The last step of particle packing is to check whether the distributed aggregates and voids intersect or overlap with each other. The straightforward, efficient but easily implemented algorithms for intersection and overlap checking of 3D spheres,
ellipsoids, polyhedrons and their different combinations are proposed in this section. In order to place an aggregate particle at a free position and orientation within the concrete volume, three conditions need to be satisfied: (1) the whole particle should be completely within the boundaries of the concrete volume; (2) there must not be any overlap with previously placed particles; (3) the minimum distance between the edge of a particle and the boundary of the concrete specimen, and the minimum gap width between two adjacent particles should be limited.

The first condition can be easily met by detecting if the minimum and maximum coordinates of the particles are inside the concrete section. The third condition can be checked concurrently with the checking of first two conditions by enlarging the size of the particle to \((1+\gamma)\) its size, where \(\gamma\) is the average film thickness. The same criterion applies to the distribution of voids in concrete. Given the set of independent and dependent parameters, the intersection and overlap checking algorithms in different situations are given below.

### 2.3.1 Random spherical inclusions

For two spherical particles, the intersection and overlapping condition can be checked easily by comparing the distance between the particle centres and the sum of two radii.

\[
\sqrt{(x' - x_o)^2 + (y' - y_o)^2 + (z' - z_o)^2} \leq r + r'
\]

where \(x'_o, y'_o, z'_o\) are the coordinates of centre of the newly generated sphere; \(r\) and \(r'\) are the radii of the previous generated and new spheres, respectively.

### 2.3.2 Random ellipsoidal inclusions

It is neither economical nor necessary to check each newly generated particle against all the existing particles for intersection and overlap checking. In order to reduce the computational cost, intersection and overlap checking is performed by using a less costly hierarchy method. The computational cost is decreased by only considering inclusions in the near field of the particles being added and excluding all the other particles in the far field.

In Hierarchy I, for two ellipsoids with centres \(A\) and \(B\), if the distance between \(A\) and \(B\) is larger than \(2a\) (\(a\) is the length of major semi principal axis), then these two ellipsoids do not intersect or overlap. Thus, all the inclusions that are at a radial distance greater than \(2a\) from the centre of the inclusion can be excluded for next
intersection and overlap checking. Consequently, no particles or very few particles need to be further checked which results in a significant increase in the computational efficiency.

Hierarchy II could further reduce the computational cost by checking whether the centres of any previously generated ellipsoids filtered in Hierarchy I are located inside or on the surface of new ellipsoid before it goes to Hierarchy III. This could make sure that the new ellipsoid does not totally contain one of the existing particles which will be ignored in Hierarchy III. Finally, Hierarchy III checks whether any nodes on new ellipsoids are located inside or on the surface of an ellipsoids filtered in Hierarchy II.

The nodes on the surface of an ellipsoid may be parameterized in several ways. One possible choice is spherical coordinate system:

\[
\begin{align*}
\bar{x} &= a \cos(\theta) \sin(\varphi) + x_0 \\
\bar{y} &= b \sin(\theta) \cos(\varphi) + y_0 \\
\bar{z} &= c \cos(\varphi) + z_0
\end{align*}
\]

where \(\theta\) is the polar angle measured from a fixed zenith direction, \(\varphi\) is the azimuth angle of its orthogonal projection on a reference plane that passes through the origin and is orthogonal to the zenith, measured from a fixed reference direction on that plane.

Considering an arbitrary node \(N(\bar{x}, \bar{y}, \bar{z})\) on an ellipsoid surface, its location relationship to another ellipsoid \(\Omega\) can be determined by calculating \(F(\bar{x}, \bar{y}, \bar{z})\):

\[
\begin{align*}
N \notin \Omega, & \quad F(\bar{x}, \bar{y}, \bar{z}) > 0 \\
N \in \Gamma_\Omega, & \quad F(\bar{x}, \bar{y}, \bar{z}) = 0 \\
N \in \Omega, & \quad F(\bar{x}, \bar{y}, \bar{z}) < 0
\end{align*}
\]

where \(\Omega\) is the ellipsoid, \(\Gamma_\Omega\) is the boundary of the ellipsoid.

If \(F(x, y, z) > 0\), then node \(N\) is at outside of the ellipsoid; if \(F(\bar{x}, \bar{y}, \bar{z}) = 0\), then node \(N\) is on the surface of the ellipsoid; if \(F(\bar{x}, \bar{y}, \bar{z}) < 0\), then node \(N\) is inside of the ellipsoid. So if any node on the surface of the newly generated ellipsoid is inside of any previous generated ellipsoids, the particle will not be placed into the model. In such a case, another set of random numbers \((a, b, c, \alpha, \beta, \gamma, x_0, y_0, z_0)\) is generated for a new ellipsoid and an attempt of placing the particle at a new location and orientation is made. Two ellipsoids are regarded as separated only when all the nodes on one ellipsoid are outside of the other one. It could be achieved by calculating \(F_i(x_0, y_0, z_0)\)
in Hierarchy II and $F_2(\bar{x}, \bar{y}, \bar{z})$ in Hierarchy III. If both $F_1(x_0, y_0, z_0)$ and $F_2(\bar{x}, \bar{y}, \bar{z})$ are positive, then the two ellipsoids are considered to be separated. The coordinates of all the nodes on the ellipsoid surface could be obtained by search algorithms in MATLAB [63].

### 2.3.3 Random polyhedral inclusions

This section discusses the method of intersection and overlap checking for convex polyhedrons. The generated random convex polyhedrons are made of the random nodes extracted from spheres. Likewise, the hierarchy algorithm as described above is used here to reduce the computational cost. So all the inclusions that are at a radial distance of the original spheres greater than $(r_1 + r_2)$ from the centre of the inclusion being added can be excluded for next intersection and overlap checking, where $r_1$ and $r_2$ are the radii of two spheres.

The method of intersection and overlap checking for polyhedrons is based on determining whether two convex polyhedrons intersect with each other. This is achieved by detecting whether all the vertexes of the existing polyhedrons lie on one side of an arbitrary plane of the new polyhedron, while any point inside the new polyhedron lie on the another side. A 3D example with polyhedron $L$ on the left and polyhedron $R$ on the right is shown in Fig. 2 to illustrate the idea of the algorithm. If all the vertexes 1-6 of polyhedron $L$ lie on the left side of the plane $ABC$ consists of vertexes $A$, $B$ and $C$, while an arbitrary point $O$ inside of the polyhedron $R$ is on the right side of the plane $ABC$, then these two polyhedrons are separated. Herein, the coordinates of arbitrary point $O$ are chosen as the mathematical mean values of all vertexes of the polyhedron.

![Fig. 2. Intersection and overlap checking for polyhedrons in 3D](image)

The equation of plane $ABC$ can be obtained with nodal coordinates denoted by $A(x_1, y_1, z_1)$, $B(x_2, y_2, z_2)$ and $C(x_3, y_3, z_3)$ as follows:
\[
\begin{bmatrix}
x & y & z & 1 \\
x_1 & y_1 & z_1 & 1 \\
x_2 & y_2 & z_2 & 1 \\
x_3 & y_3 & z_3 & 1 \\
\end{bmatrix} = 0
\]  
(6)

So the general equation of plane \(ABC\) can be expressed as:

\[
G(x, y, z) = (x-x_1) \begin{bmatrix} y_2-y_1 & z_2-z_1 \\ y_3-y_1 & z_3-z_1 \end{bmatrix} + (y-y_1) \begin{bmatrix} z_2-z_1 & x_2-x_1 \\ z_3-z_1 & x_3-x_1 \end{bmatrix} + (z-z_1) \begin{bmatrix} x_2-x_1 & y_2-y_1 \\ x_3-x_1 & y_3-y_1 \end{bmatrix}
\]  
(7)

Considering all the vertices \(N(x_v, y_v, z_v)\) on polyhedron \(L\) and the point \(O(x_o, y_o, z_o)\) inside polyhedron \(R\), the location of point \(N\) relative to the polyhedron \(R\) can be determined by calculating \(G(x_v, y_v, z_v) \times G(x_o, y_o, z_o)\). If \(G(x_v, y_v, z_v) \times G(x_o, y_o, z_o)<0\) for all the vertexes, then these two polyhedrons are considered to be separate.

2.3.4 Random spherical/ellipsoidal inclusions and random spherical/ellipsoidal voids

The first hierarchy algorithm that a radial distance of the sphere and ellipsoid greater than \((r+a)\) from the centre of the inclusions being added can be excluded for the next intersection and overlap checking, is used. The general equation of a sphere can be expressed by the standard equation (see Equation (A1) in Appendix):

\[
H(x, y, z) = Ax^2 + By^2 + Cz^2 + Dx + Ey + Fz + G \leq 0
\]  
(8)

The surface of a sphere can be parameterized using spherical coordinates \((r, \theta, \phi)\):

\[
\begin{align*}
    r &= r_0 + \eta \times (r_1 - r_0) \\
    \theta &= \eta \times 2\pi \\
    \phi &= \eta \times \pi
\end{align*}
\]  
(9)

where \(\theta\) and \(\phi\) have the same meaning as those given in Equation (4), \(r_0\) and \(r_1\) are the minimum and maximum radii of particle, \(\eta\) denotes a random number uniformly distributed between 0 and 1.

Like those for ellipsoids, the intersection and overlap between ellipsoids and spheres can be evaluated by checking whether all the nodes on an ellipsoid/sphere are outside of the other sphere/ellipsoid. Considering all nodes \(N(x_n, y_n, z_n)\) on a sphere/ellipsoid, their location relative to another ellipsoid/sphere can be determined by \(F(x_n, y_n, z_n)\) or \(H(x_n, y_n, z_n)\). If \(F(x_n, y_n, z_n)>0\) or \(H(x_n, y_n, z_n)>0\) for all the vertexes, then the sphere and ellipsoid are regarded as separate ones. Meanwhile, Hierarchy II is performed to make sure that the new sphere/ellipsoid does not contain the previous ones, the centres of which may be inside or on the surface of the new particle.
2.3.5 Random polyhedral inclusions and random spherical/ellipsoidal voids

The first hierarchy algorithm similar to the previous one but with different region range, \((r+r')\) for polyhedron and sphere, and \((r+a)\) for polyhedron and ellipsoid, is used. The further checking is carried out by using the similar method as that used for polyhedrons as described above, but all nodes on the surfaces of spheres/ellipsoids are regarded as vertexes. Here the spheres or ellipsoids are assumed to be generated before the polyhedrons. Considering all nodes \(N(x_n, y_n, z_n)\) on a sphere/ellipsoid and the point \(O(x_o, y_o, z_o)\) inside of the polyhedron, the sphere/ellipsoid location relative to the polyhedron can be determined by \(H(x_n, y_n, z_n)\times G(x_o, y_o, z_o)\) or \(G(x_n, y_n, z_n)\times G(x_o, y_o, z_o)\). If \(H(x_n, y_n, z_n)\times G(x_o, y_o, z_o)<0\) or \(G(x_n, y_n, z_n)\times G(x_o, y_o, z_o)<0\) for all nodes, then the polyhedron and sphere/ellipsoid are regarded as separate ones.

2.4 Meso-structure models

2.4.1 Concrete with gravel aggregates

Based on the developed particle generation and packing procedure, a series of cubic concrete samples with dimensions of 50mm×50mm×50mm containing spherical and ellipsoidal gravel aggregates and voids are generated, as shown in Fig. 3, where aggregates are in green and voids are in red. The other phase in the cube represents mortar. The used aggregate size distribution is given in Table 1. The aspect ratios for ellipsoidal aggregates and voids are \(R_1=R_2=[1, 2]\). The minimum thickness of the mortar film around the aggregates is a challenge, because no simple theory is available yet for its evaluation. The thickness was assumed to be 0.1-1mm in most of the previous numerical studies \([64, 65]\). Although it has been found to have an insignificant effect on the concrete behaviour \([64]\), it plays an important role in the spatial distribution of the aggregate particles: a larger value would result in a more uniform spatial distribution but could lead to the limit for reaching a high volume fraction. In present study, the minimum space between the edge of an aggregate and the boundary of the concrete specimen \((\gamma_1)\), and minimum gap width between any two aggregates \((\gamma_2)\) are set to be 0.2 mm, as recommended in \([62]\).

Concrete specimens composed of spherical gravel aggregates with volume fraction \((P_{agg})\) of 30% and spherical/ellipsoidal voids with volume fraction \((P_{void})\) of 0% and 2% are shown in Fig. 3(a), Fig. 3(b) and Fig. 3(c), respectively. Concrete specimens made up of ellipsoidal gravel aggregates with volume fraction of 30% and spherical/ellipsoidal voids with volume fraction of 0% and 2% are shown in Fig. 3(d), Fig. 3(e) and Fig. 3(f), respectively.
Fig. 3. 3D mesostructures of concrete with gravel aggregates ($P_{agg}=30\%$) and voids ($P_{void}=0\%, 2\%$).

Fig. 4 shows the generated 3D meso-structures of concrete with 2% spherical voids and ellipsoidal gravel aggregates, the volume fraction of which is 15%, 25% and 35%, respectively. The meso-structures of concrete with 30% ellipsoidal aggregates and different void content (i.e., 1%, 3% and 6%) are shown in Fig. 5. Fig. 6 illustrates the meso-structures of concrete specimens with 2% spherical voids and ellipsoidal aggregates ($P_{agg}=30\%$), the aspect ratios $R_1$ and $R_2$ of which range from $[1, 1.5], [2, 2.5]$ to $[3, 3.5]$. 

Fig. 4. Meso-structures of concrete with different aggregate volume fraction (ellipsoidal aggregates and spherical voids, $P_{void}=2\%$)
2.4.2 Concrete with crushed aggregates

Polyhedral aggregates and spherical or ellipsoidal voids are considered for concrete with crushed aggregates. A series of 3D cubic concrete samples (50mm×50mm×50mm) consisting of mortar, polyhedral crushed aggregates and spherical/ellipsoidal voids are generated and shown in Fig. 7. The minimum and maximum edges of the polyhedrons are set to $M_{\text{min}}=8$, $M_{\text{max}}=16$. All other parameters are the same as those used for concrete with gravel aggregates above.
2.4.3 Efficiency of the proposed algorithm

In order to investigate the quality of the proposed hierarchy algorithm, the computational times involved in generating typical unit cells (50mm×50mm×50mm) with ellipsoidal particles ($P_{agg}=20\%$) and spherical voids ($P_{void}=1\%$) by employing the present proposed algorithm and generally used traditional algorithm are shown in Fig. 8. These simulations were performed using an Intel Core i7 @ 3.4 GHz desktop computer with 8 GB RAM. It is evident that the present algorithm significantly reduces computational cost as compared to the traditional algorithm, with mean computational time 16.2s for the present algorithm and 515.8s for the traditional algorithm.

![Fig. 8. Comparison of CPU times between two algorithms](image)

3 Finite element modelling

3.1 Mesh generation

The generated meso-structures of concrete as illustrated in Section 2 are subsequently meshed for modelling with cohesive elements. In this work, all finite element meshing are performed with the pre-processing functionality in commercial FE package ANSYS [66]. The free meshing technique with mesh adaptation functions was used to avoid the restriction on model geometry. For meshing, different components in concrete, e.g., mortar and aggregates should maintain continuity on their surfaces. Thus, the finite element boundaries are coincident with material surfaces and there are no material discontinuities within the elements. The detailed meshing procedure is described as follows:
Firstly, the entire concrete volume $V_{all}$ and the volume representing aggregates $V_{agg}$ are created. The “overlapping” Boolean operation in the ANSYS pre-processor is applied to separate aggregates from entire domain. The remaining volume belongs to mortar and voids, denoted by $V_{mix}$. Secondly, the volume representing voids $V_{void}$ is created, and the “overlapping” Boolean operation is utilized again to separate $V_{void}$ from $V_{mix}$. The remaining volume is mortar, denoted as $V_{mortar}$. Finally, the volume representing voids is deleted, since voids do not contribute to macroscopic mechanical properties of concrete.

The mortar and aggregates are meshed with tetrahedral elements so that more realistic crack paths can be obtained. The ANSYS parametric design language (APDL) programs in combination with ANSYS batch processing are developed to provide a powerful tool of automatic mesh generation for a large number of samples required for Monte Carlo simulation.

### 3.2 Cohesive element insertion

After finite element meshing, the generated mesh will automatically have shared nodes at the interfaces between two elements. A duplicate set of nodes is required at the interfaces in order to simulate the potential micro-crack initiation in cohesive zone model. Here 6-node zero in-plane thickness cohesive interface elements (CIEs) are pre-inserted into the existing element surfaces. This is implemented by using an in-house computer program CIEIN, which is programmed in FORTRAN [67].

An example of cohesive interface element inserting into the surface between aggregate and mortar is shown in Fig. 8, where three sets of CIEs with different traction-separation softening laws, namely, CIE_AGG, CIE_MOR and CIE_INT are assigned to aggregate, mortar and interface, respectively. As a result, Fig.8(a) and Fig.8(b) show the initial FE mesh (4 elements and 7 nodes) is changed into FE mesh with inserted cohesive elements (7 elements, 15 nodes). The entire procedure for interface elements inserting into finite element mesh is described in detail below:

1. Reading the original mesh file generated from ANSYS including information on element (nodal connectivity), node (nodal coordinate) and material numbering (1 for aggregate and 2 for mortar);

2. Every normal node between each pair of solid elements (i.e., aggregate and mortar) is duplicated so that a separated node is created in the same position for every two adjacent elements. The nodal connectivity is changed by using these duplicated
nodes, which results in each element being not connected with its neighbouring elements;

(3) Inserting three different zero-thickness cohesive interface elements (CIEs) with distinct mechanical properties, namely CIE_AGG, CIE_MOR, and CIE_INT into aggregate-aggregate, mortar-mortar, mortar-aggregate interfaces, respectively. As a result, all solid elements are connected with each other again;

(4) Generating a new input file in INP format for ABAQUS by updating the mesh information of solid elements C3D4_AGG for aggregate, C3D4_MOR for mortar, and three cohesive interface elements CIE_AGG, CIE_MOR, and CIE_INT for interfaces.

A loop algorithm has been developed to generate every INP file including information of material properties, boundary and loading conditions for ABAQUS in combination with the mesh files automatically obtained from ANSYS.

A typical finite element model including cohesive interface elements for cubic concrete specimen with 30% ellipsoidal aggregates and 2% spherical voids is taken as an example and shown in Fig. 9. Different phases made of meso-structure of concrete, i.e., aggregate, void and mortar, are identified and meshed firstly, as shown in Fig. 9(a). Three sets of cohesive interface elements, i.e., CIE_AGG, CIE_MOR and CIE_INT are then respectively inserted into the initial mesh, as shown in Fig. 10(b), (c) and (d).
3.3 Cohesive interface constitutive behaviour

The behaviour of zero-thickness cohesive elements is given with a relation between surface traction (stress) and separation (displacement between originally coinciding surfaces). In 3D cohesive zone model, it is generally assumed that there exist a normal traction $t_n$ and two tangential traction (shear cohesion) $t_s$ and $t_t$ across the crack surfaces, through mechanisms such as material bonding, aggregate interlocking and surface friction in fracture process zone. The traction-separation relation has two distinct phases: (1) surfaces maintain full integrity; and (2) surfaces gradually separate to complete loss of interaction. For quasi-brittle materials, such as the concrete constituents, mortar and aggregate, phase (1) can be assumed linear elastic. The critical point between the two phases, called the damage initiation point, can be defined in terms of either critical traction or critical separation. In this study, critical points are defined in terms of critical tractions for the three modes, $t_{n0}$, $t_{s0}$ and $t_{t0}$, respectively, and the element damage initiates when the following condition is met

$$\left\{ \frac{t_n}{t_{n0}} \right\}^2 + \left\{ \frac{t_s}{t_{s0}} \right\}^2 + \left\{ \frac{t_t}{t_{t0}} \right\}^2 = 1$$

(10)

For the separation phase (2), we have selected a linear-softening response, i.e. the traction decreases linearly with the separation beyond the critical. This leads to bilinear cohesive crack model, illustrated in Fig. 10 for normal and tangential separations. In the figure, $\delta_{n0}$ and $\delta_{s0}(\delta_{t0})$ denote the critical separations, corresponding to the critical tractions $t_{n0}$, $t_{s0}$ and $t_{t0}$, respectively, and $\delta_{nf}$ and $\delta_{sf}(\delta_{tf})$ denote the separations at complete failure for normal traction and tangential traction, respectively. The unloading paths are also indicated. The initial stiffness $k_{n0}$, $k_{s0}$ and $k_{t0}$ must be set high enough to minimize an overly-flexible response in cohesive zone system, but not
too high to produce instabilities in the stiffness matrix. This is because the compliance due to the presence of interfaces should be negligible compared with the compliance of continuum elements; they represent the potential crack paths in a physical sense. Meanwhile, it should be noted that excessively high values may lead to ill-conditioning of the system equations and low values cannot ensure displacement continuity across the interfaces in the elastic range. The effects of initial stiffness on computational results have been investigated previously [68, 69]. The following relation is suggested in [69] as a guideline for initial stiffness selection:

\[
k_n = k_s = \frac{c(1-v)}{b(1+v)(1-2v)}E
\]

where \(E\) and \(v\) are Young’s modulus and Poisson’s ratio, \(b\) is the characteristic size of elements, and \(c\) is taken as 10-100 from the experience in Qiang et al. [69]. An appropriate elastic stiffness of the interfaces equal to \(10^6\) MPa/mm is chosen as used in 2D models [11, 13] and 3D studies [36].

The areas under the curves respectively stand for the normal fracture energy and tangential fracture energy \(G_{nf}(G_{t0})\). These are related to the tensile/shear strength and failure separation according to

\[
G = \int_{\delta_f}^{\delta} t(\delta)d\delta = \frac{1}{2} t_0 \delta_f
\]

Hence knowledge of two of the parameters, \(G\), \(t_0\) and \(\delta_f\), fully determines the traction separation law. In this work we have used knowledge of fracture energies and critical tractions from previous works.

Fig. 11. Traction-separation laws for cohesive interface elements
The evolution of damage in phase (2) under the combined normal and tangential separations is described via a scalar index $D$. To this end an effective relative displacements $\delta_m$, introduced as

$$\delta_m = \sqrt{\langle \delta_n \rangle^2 + \delta_s^2 + \delta_t^2}$$  \hspace{1cm} (13)

where $\langle >$ is the Macaulay bracket

$$< \delta_n >= \begin{cases} \delta_n , & \delta_n \geq 0 \text{ (tension)} \\ 0 , & \delta_n < 0 \text{ (compression)} \end{cases}$$  \hspace{1cm} (14)

is used to define the scalar damage

$$D = \frac{\delta_{m,f} (\delta_{m,\text{max}} - \delta_{m,0})}{\delta_{m,\text{max}} (\delta_{m,f} - \delta_{m,0})}$$  \hspace{1cm} (15)

where $\delta_{m,\text{max}}$ is the maximum effective relative displacement obtained during the loading history, $\delta_{m,0}$ and $\delta_{m,f}$ denote the effective relative displacements at damage initiation and final failure, respectively. Notably, the damage variable $D$ evolves monotonically from 0 to 1 during loading.

Damage evolution affects the stiffness coefficients $k_n$, $k_s$ and $k_t$ for unloading and reloading, which change according to

$$k_n = (1-D)k_{n,0}, \quad k_s = (1-D)k_{s,0}, \quad k_t = (1-D)k_{t,0}$$  \hspace{1cm} (16)

This affects the tractions, which change according to

$$t_n = \begin{cases} (1-D)\tilde{t}_n , & \tilde{t}_n \geq 0 \\ \tilde{t}_n , & \tilde{t}_n < 0 \end{cases}$$  \hspace{1cm} (17)

$$t_s = (1-D)\tilde{t}_s$$

$$t_t = (1-D)\tilde{t}_t$$  \hspace{1cm} (18)

where $\tilde{t}_n$, $\tilde{t}_s$ and $\tilde{t}_t$ are the traction components predicted by the elastic traction-displacement behaviour for the current separation without damage. The theoretical framework described above is used for the intra-phase and inter-phase cohesive elements in the meso-structure with different parameters for mortar-mortar, mortar-aggregate and aggregate-aggregate boundaries.

The constitutive laws selected for CIEs in this study are primarily for modelling interface fracture, and do not represent fully the coupling between shear and normal responses, particularly the interaction between shear and compression. It is expected that this simplification has minor effect on the analysis of concrete under uniaxial tension in the pre-peak regime dominated by tensile micro-cracking. The effect on the post-peak behaviour, governed by micro-crack coalescence and associated
development of shear failures, might be captured less accurately. In order to accommodate general loading conditions, specific cohesive models are required to incorporate the mechanism that the shear strength is highly dependent on the normal stress at the interfaces. Such models, based on finite-thickness cohesive elements are under development.

### 3.4 Model description for Monte Carlo analysis

All models analysed in this work have dimensions of 25mm×25mm×25mm. For a given set of meso-structure characteristics (aggregate and void content, shape and size distribution, etc.), a number of model realisations differing in the spatial distributions of these features, have been generated for the purposes of subsequent statistical analysis of the macroscopic responses. Simulations with the realisations corresponding to a fixed set of meso-structure parameters constitute a Monte Carlo analysis of the set.

The mechanical properties of the two phases in concrete as well as the properties of the interface elements used in this work, obtained from [36], are given in Table 2. Regarding the aggregate-aggregate interfaces (CIE_AGG), it is noted that aggregates have much higher strength than mortar-mortar (CIE_MOR) and mortar-aggregate interfaces (CIE_INT) in normal concrete. Therefore, cracks are normally not allowed to initiate inside aggregates unless otherwise specified. This is implemented by defining elastic behaviour without damage for CIE_AGG. Due to lack of experimental data, the shear fracture properties were assumed to be the same as the normal ones [13, 14] for both CIE_MOR and CIE_INT. The linear tension/shear softening laws described in Section 3.3 are used to model these interfaces.

<table>
<thead>
<tr>
<th>Material</th>
<th>Young’s modulus E (MPa)</th>
<th>Poisson’s ratio ν</th>
<th>Density ρ (10⁹ tone/mm³)</th>
<th>Elastic stiffness kₙ (MPa/mm)</th>
<th>Cohesive strength t₀ (MPa)</th>
<th>Fracture energy Gₕ (N/mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aggregate</td>
<td>70000</td>
<td>0.2</td>
<td>2.8</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>Mortar</td>
<td>25000</td>
<td>0.2</td>
<td>2.0</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>CIE_AGG</td>
<td>–</td>
<td>–</td>
<td>2.8</td>
<td>10⁶</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>CIE_MOR</td>
<td>–</td>
<td>–</td>
<td>2.5</td>
<td>10⁶</td>
<td>4</td>
<td>0.06</td>
</tr>
<tr>
<td>CIE_INT</td>
<td>–</td>
<td>–</td>
<td>2.0</td>
<td>10⁶</td>
<td>2</td>
<td>0.03</td>
</tr>
</tbody>
</table>

The loading on all model specimens has been applied via prescribed displacement, where horizontal displacements were prescribed to all nodes on the left and right
surfaces, with a value equal to zero for the left surface, and a uniformly distributed displacement on the right surface. The analyses were terminated at a displacement $d=0.1$ mm, corresponding to macroscopic strain of $\varepsilon=0.002$, the same as those used in our previous 2D study [13]. The ABAQUS/Implicit solver using the default automatic incrementing often fails to finish the whole modelling for highly nonlinear problems with material softening. A very small value of the maximum increment is required to model the whole loading process, while it will lead to a high computational cost. The Dynamic/Explicit solver with long enough loading time to minimize the dynamic effect is able to predict the full curve accurately with a reasonable time and thus is used in this study. Therefore, solutions were performed with the commercial software ABAQUS/Explicit, it determines a solution to the dynamic equilibrium equation without iterating by explicitly advancing the kinematic state from the previous increment, which allows for solving highly nonlinear equation systems with softening-induced instabilities.

4 Results and discussion

4.1 Analysis of simulation parameters

Cohesive zone models are known to produce results affected by element size and, in the case of dynamic analysis, such as in Abaqus/Explicit, by loading time. This sub-section presents an advance study of these effects to inform on most appropriate size and time. Further the effect of Monte Carlo sample number, i.e. number of realisations per fixed set of meso-structure parameters, is analysed. The outcomes are summarised as those used for the parametric studies in the following sub-sections.

4.1.1 Effect of mesh density/element size

When the cohesive crack paths are unknown a priori, fine meshes are needed to minimise the dependence of simulation results, e.g., stress-displacement curves and crack patterns, on initial FE mesh. However, this will lead to large-scale nonlinear equation systems, and the computational costs often become prohibitively expensive, especially for Monte Carlo simulations. Moreover, the effect of the minimum thickness around aggregates may potentially be related to the global mesh size. Therefore, an appropriate mesh density is required to achieve a balance between the accuracy and computational efficiency. Herein, three meshes with different average element length (i.e., $L_e=1$ mm, $L_e=0.8$ mm and $L_e=0.6$ mm) are used, as shown in Fig.
11. Mesh I has 156241 nodes, 28432 solid elements and 307475 cohesive elements. The numbers for the meshes II and III are 236,260, 42,714 and 465,435, and 349,777, 62,466 and 690,464, respectively.

Fig. 12. Three different mesh configurations with different mesh density

The simulated stress-displacement ($\sigma$-$d$) and dissipated fracture energy-displacement curves for each element length are shown in Fig. 12, where the mean stress is calculated as the sum of reaction force of nodes on the left boundary divided by the cross-sectional area of specimen. It can be observed that the mesh dependence of the stress-displacement and dissipated fracture energy-displacement curves is negligible for the selected element sizes.

The obtained final crack paths for different meshes are shown in Fig. 13 to Fig. 15, where plots (a) represent the failure surfaces and plots (b) represent the damage via the separations of the cohesive elements with damage index $D\geq0.95$, where $D=1$ means complete failure, are shown in red. Despite a few differences, the three figures show similarity in terms of crack pattern and failed surface morphology. Considering the excellent agreement between the stress-displacement responses in Fig. 12, and the balance between accuracy and efficiency, the mesh size of 1mm (Mesh I) has been selected for all meshes in the following simulations.

Fig. 13. Mesh sensitivity results
4.1.2 Effect of loading time

The loading time has a significant effect on the computational efficiency and accuracy of results when the ABAQUS/ Explicit solver is used to model quasi-static loading conditions. In principle, the loading time must be long enough to minimise any dynamic effects. However, a long loading time results in greater computational cost. So a balance also has to be made between the computational efficiency and accuracy.
Fig. 16 shows a comparison of $\sigma$-$d$ curves obtained from 50 random samples with three loading times of 0.001s, 0.005s and 0.01s. It can be seen that a loading rate influence occurs when loading time is 0.001s (a), and there is an obvious oscillation. For loading rates 0.005s (b) and 0.01s (c), the curves appear smooth and identical. A loading time of 0.005s is used in the following simulations to balance efficiency and accuracy.

(a) Loading time=0.001s  (b) Loading time=0.005s  (c) Loading time=0.01s

Fig. 17. Effect of loading time on stress-displacement curves

4.1.3 Typical tensile behaviour

3D modelling allows for more realistic representation of aggregate and void distribution in concrete compared to previous 2D models. The need for statistical representativeness requires a significant number of model realizations per set of mesostructure parameters to ensure convergence. This makes the Monte Carlo approach substantially more computationally demanding in 3D and requires some balance between number of realizations and available computer power.

Stress-displacement curves from a Monte Carlo simulation with 50 realisations are shown in Fig. 17 together with the numerical mean curve and experimental data acquired from tension tests of six samples by Hordijk [62]. The simulated stress-displacement curves in this work fit well with the experimental scatter. They are similar in terms of clear peak and sharp initial post-peak drop followed by a long shallow tail. The peak stress has a mean of 3.49 MPa with standard deviation of 0.05 MPa, demonstrating that it is relatively insensitive to the spatial randomness of aggregates and voids. However, notably large differences are observed between the softening responses of the different realisations. This suggests that sufficient number of realisations is necessary to capture a required accuracy. In order to select suitable points for comparison between different numbers of realisations, the standard deviation of stress during loading is plotted in Fig. 18. The standard deviation of stress is relatively low (around 0.05MPa) before it reaches the peak stress.
(displacement=0.01mm), and the deviation first increases to around 0.5MPa and then decreases.

![Fig. 18. Stress-displacement curves obtained from Monte Carlo simulation](image)

![Fig. 19. Standard deviation of stress with displacement](image)

4.1.4 Effect of sample number

In order to evaluate the effect of Monte Carlo sample number on simulation results, two special loading points, corresponding to the peak stress and the displacement of 0.03mm when the highest standard deviation is observed during loading process (Fig. 18), are investigated, the results are shown in Fig. 19 and Fig. 20, respectively. Both the mean value and standard deviation of stress tend to be stable when the sample number is about 50, which indicates that 50 random samples are enough to achieve statistical convergence. It should also be noted that Gaussian distribution was found in Wang and Jivkov [70] for peak stress which indicates the stress distribution is not completely random, however, substantially more samples are necessary to yield conclusive results for softening behaviour due to the relatively high coefficient of variance of stress (standard deviation/mean value).

![Fig. 20. Effect of the sample number on the peak stress](image)

![Fig. 21. Effect of the sample number on stress at displacement=0.03](image)

Monte Carlo simulations with 50 realisations per set of parameters were carried out in this study using the High Performance Computing (HPC) cluster at
A typical Monte Carlo analysis of 50 realisations using the mesh size of 1 mm and loading time of 0.005s took approximately 6 hours by ABAQUS default parallel processing with 32 CPUs.

4.1.5 **Comparison with 2D models**

As mentioned in the introduction, most of existing work on meso-scale modelling of damage and failure of concrete is performed with 2D models (plane stress). It is therefore interesting to assess the difference between the responses of 2D and 3D meso-structures. To this end, 50 2D models of concrete with elliptical aggregates and circular voids were generated using the algorithms from Wang et al. [13]. All meso-scale parameters were fixed to the values used in the 3D model described in section 3.4. Afterwards, Monte Carlo simulations are carried out to estimate the mechanical behaviour of these 2D concrete samples under uniaxial tension. The emergent stress-displacement curves together with the mean curve are shown in Fig. 21.

For comparison, the mean responses from 2D and 3D simulations are given together in Fig. 22. The mean peak stresses predicted by 2D and 3D modelling are 2.65 MPa and 3.49 MPa, respectively, i.e. the more realistic 3D meso-structure predicts 24.1% higher peak stress. The standard deviations of peak stress are 0.11 MPa and 0.05 MPa, respectively, i.e. the 3D model provide 54.5% lower standard deviation. In the softening phase of the responses, the 3D models show generally larger standard deviation of stress than the 2D models. The increase of peak stress in 3D is attributed to the constraint effect in the thickness direction, not captured by the 2D model. The decrease of standard deviation of peak stress is attributed to the larger ratio between surfaces available for cracking and volume in 3D than line segments available for cracking and area in 2D. This leads to more uniformly distributed pre-peak micro-cracks in the 3D volume. The outcome is that the spatial distribution of features has substantially weaker effect on the pre-peak response in the 3D models than in the 2D models. In the softening branch, the larger standard deviation of stress predicted by the 3D models is related to the process of micro-crack coalescences into macroscopic cracks. Here the more uniformly distributed micro-cracks from the pre-peak phase in 3D have significantly more options to coalesce depending on the spatial distribution of the features. As a result, the spatial distribution of features guiding
micro-crack coalescence has substantially stronger effect on the post-peak response in the 3D models than in the 2D models.

The results presented suggest that the use of 2D approximation can bring significant underestimation of strength and toughness of concrete, where toughness is understood as the area under the stress-strain curve. Clearly, the third dimension cannot be neglected due to the nature of fracture process. The importance of the thickness effect has been pointed out experimentally by Van Mier and Schlangen [71].

![Graph](image)

**Fig. 22.** Comparison of 2D and 3D modelling

### 4.2 Crack patterns

Two typical macro-crack patterns are observed from the Monte Carlo simulations under uniaxial tension: Type I cracking with only one dominant crack illustrated in Fig. 23; and Type II cracking with two or more dominant cracks illustrated in Fig. 24. This finding is consistent with that observed by Roubin [72] via image-based modelling, as shown in Fig. 25. Figures 23 and 24 present the crack patterns at four loading stages. To clearly visualise the fracture surfaces, three different ways are used: models with damaged cohesive elements (left column, displacement magnification factor of 20), model without cohesive elements (middle column, displacement magnification factor of 200) and failed interfaces only (right column, displacement magnification factor of 20).

The damage index is represented in red colour. In the early stages of loading, a large number of micro-cracks initiate at mortar-aggregate interfaces. As loading increases, some cracks coalesce into the dominant cracks, while the other cracks arrest due to stress redistribution. Type I cracking arises when micro-cracks coalesce into a single dominant crack. Type II cracking occurs when two or more independent cracks form during the coalescence process.
Fig. 23. Typical Type I cracking evolutions at various loading stages shown in models with CIEs (left column), models without CIEs (middle column) and cracked interfaces (right column)
Fig. 24. Typical Type II cracking evolutions at various loading stages shown in models with CIEs (left column), models without CIEs (middle column) and cracked interfaces (right column)
Fig. 25. Two typical types of cracking in concrete under tension obtained from image-based modelling (after [72])

Fig. 26 shows the stress-displacement curves corresponding to two different types of cracking, red dashed lines for Type I cracking and blue solid lines for Type II cracking. Among 50 Monte Carlo samples investigated in this particular study, 38 samples behave as Type I cracking and 12 samples behave as Type II cracking. It can be seen that, there is an almost identical response of monotonous increase in the pre-peak range. For both Type I and Type II, the average peak stress is very close to each other, about 3.50 MPa. However, a clear difference is observed between the post-peak responses.

Fig. 26. Comparison of stress-displacement curves for different types of cracking (For interpretation of the references to colour in this figure, the readers is referred to the web version of this article)
If a single crack develops (Fig. 23), the stress-displacement curve presents a rapid softening (see red curves in Fig. 26). If two or more macro-cracks form concurrently (Fig. 24), the softening is more graceful (see blue curves in Fig. 26). This indicates that the post-peak softening is related to cracking type. The emergence of multiple concurrently growing macro-cracks leads to larger apparent toughness of the representative volume analysed.

4.3 Analysis of meso-structure parameters effects

4.3.1 Effect of aggregate and void content

Based on Monte Carlo simulations, the effect of aggregate content is investigated. All the parameters except for aggregate volume fraction are fixed to the values used in Section 3.4. Fig. 27(a) shows the mean stress-displacement curves for samples with different aggregate volume fractions. The corresponding mean peak stress against aggregate volume fraction is plotted in Fig. 27(b). It can be observed that the mean load carrying capacity decreases 14% in strength, from 3.99 MPa to 3.49 MPa, with the increase of aggregate volume fraction from 0% to 30%. This is because the increase of weak aggregate-mortar interfaces has a greater influence than the increase in strong aggregates as the cohesive strength of interfacial CIEs is assumed to be only half of mortar CIEs in this study.

![Stress-displacement curves](image1)

(a) Stress-displacement curves

![Peak stress](image2)

(b) Peak stress

Fig. 27. Effects of aggregate volume fraction ($P_{\text{agg}}=0\%$)

Fig. 28 shows the effect of void content on the concrete response. The mean tensile strength decreases from 3.59 MPa to 3.39 MPa, as the void content increases from 0% to 4%. This is attributed to the fact that the voids provide easier pathways for crack propagation. Although the differences observed for void contents rising from 0% to 4% are not significant, the results indicate that the voids existing in concrete should not be neglected in modelling of mechanical properties and fracture of concrete, in particular for concrete with high void content, such as porous concrete.
4.3.2 Effect of aggregate and void shape

The effect of aggregate and void shape is investigated by undertaking 50 Monte Carlo simulations with varying aggregate and void shape while all other parameters are fixed to those used in Section 3.4. Fig. 29 illustrates two typical crack types observed in concrete with spherical/polyhedral aggregates and ellipsoidal voids. Both types of cracking can be found in concrete samples with different shape of aggregates and voids. This suggests that the type of cracking is independent of aggregate and void shape.

Fig. 29. Typical type I and type II cracking paths for samples with different aggregate and void shape (displacement magnification factor of 200)

Fig. 30 shows the simulated mean stress-displacement curves for concrete samples with different aggregate and void shape under uniaxial tension. The results indicate that the load-carrying capacity of concrete containing spherical and ellipsoidal aggregates is greater than that including polyhedral aggregates. The difference of tensile strength between samples with spherical aggregates and elliptical aggregates is about 1% while its difference between samples with spherical aggregates and polyhedral aggregates is about 3%. This may be explained by two factors. On the one hand, concrete with unsmooth aggregates has more mortar-aggregate interface elements if aggregate and void content are constant. This is
presented in Table 3. On the other hand, the local stresses are enhanced by the higher stress concentration at the corners of polyhedral aggregates, while the smooth edges of spherical and ellipsoidal aggregates have a more benign stress distribution which delays the fracture process and increases the tensile strength.

![Graph showing mean stress vs. displacement for different aggregate and void shapes.](image)

**Fig. 30. Effect of aggregate and void shape**

<table>
<thead>
<tr>
<th>Shape</th>
<th>Aggregate-mortar interface element number</th>
<th>Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spherical aggregates and spherical voids</td>
<td>8260</td>
<td>–</td>
</tr>
<tr>
<td>Spherical aggregates and ellipsoidal voids</td>
<td>8608</td>
<td>1.04</td>
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<tr>
<td>Ellipsoidal aggregates and spherical voids</td>
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</tr>
<tr>
<td>Polyhedral aggregates and spherical voids</td>
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</tr>
<tr>
<td>Polyhedral aggregates and ellipsoidal voids</td>
<td>15,446</td>
<td>1.87</td>
</tr>
</tbody>
</table>

### 4.4 Analysis of cohesive interface effects

In this sub-section, the effect of principal material parameters, critical tensile stress and cohesive energy, used for aggregate-aggregate, mortar-mortar and mortar-aggregate interface elements on the simulation results are investigated. All other geometric parameters are fixed to those used in Section 3.4.

#### 4.4.1 Effect of critical tensile stress

Fig. 31, Fig. 33 and Fig. 35 present the simulation results obtained by varying the critical tensile stress of interface elements. For each curve in the figures, the legend includes three values, which correspond to the critical tensile stress assigned to the mortar-aggregate, aggregate-aggregate and mortar-mortar interfaces, respectively. A missing value for the aggregate-aggregate critical tensile stress indicates that cracking of the aggregate is not allowed.
It can be seen from Fig. 31 that the load carrying capacity is greatly affected by the critical tensile stress of mortar-aggregate interfaces. The decrease of tensile stress of aggregate-mortar interfaces leads to a rapid loss of load carrying capacity. This is because the aggregate-mortar interfaces are weak relative to aggregates and mortar, and become preferred crack paths. Fig. 32 shows the predicted crack paths for different critical tensile stress of mortar-aggregate interfaces. At the lowest stress of 1 MPa of mortar-aggregate interface, the crack path appears to be along mortar-aggregate interfaces. For higher mortar-aggregate interface critical tensile stress, the crack paths tend to be independent of the critical tensile stress of mortar-aggregate interfaces.

Fig. 31. Effect of critical tensile stress of mortar-aggregate interfaces

Fig. 32. Crack surfaces with different tensile strength of mortar-aggregate interfaces
Fig. 33 shows that the load carrying capacity is hardly affected by the critical tensile stress of the aggregate-aggregate interfaces until it becomes equal to the strength of mortar-aggregate interfaces. This is because aggregates are stronger than mortar and interfaces, and the load carrying capacity is not sensitive to the tensile strength of aggregates. The crack paths for different tensile strength of aggregate-aggregate interfaces are shown in Fig. 34. It can be seen that, as the aggregate strength is reduced, cracks seem to have a greater tendency to propagate across the aggregates leading to straighter paths with less bridging and branching.

Fig. 33. Effect of critical tensile stress of aggregate-aggregate interfaces

(a) \( t_n = 2 \) MPa  
(b) \( t_n = 4 \) MPa

Fig. 34. Crack surfaces with different tensile strength of aggregate-aggregate interfaces

Fig. 35 illustrates that the tensile strength of mortar-mortar interfaces has a significant influence on the load carrying capacity of concrete samples. The decrease of tensile strength of mortar-mortar interfaces results in a rapidly falling load carrying capacity. Fig. 36 shows the crack paths corresponding to different tensile strength of mortar-mortar interfaces. The cracks show a tendency to bypass the aggregates and propagate in a straight path through mortar and voids when the tensile strength of mortar-mortar interfaces is the same as that of mortar-aggregate interfaces, Fig. 36(a).
This is because the mortar-aggregate interfaces are no longer the weakest part. However, the crack paths seem to be insensitive to the tensile strength of mortar-mortar interfaces when the mortar is strong.

![Fig. 35. Effect of critical tensile stress of mortar-mortar interfaces](image)

4.4.2 Effect of cohesive energy

Fig. 37, Fig. 39 and Fig. 41 depict the simulation results obtained by varying the cohesive energy of interface elements. For each curve in the figures, the legend includes three values, which denote the cohesive energy assigned to the mortar-aggregate, aggregate-aggregate and mortar-mortar interfaces, respectively. As in the previous sub-section, a missing value for the aggregate-aggregate interface indicates that cracking through aggregates is not allowed.

It can be seen from Fig. 37, that the cohesive energy of mortar-aggregate interfaces has a significant effect on the softening response of the concrete. Fig. 38 shows the predicted crack paths for different cohesive energy of mortar-mortar interfaces. It indicates that the crack paths are dependent on the cohesive energy of mortar-aggregate interfaces.
Fig. 37. Effect of cohesive energy of mortar-aggregate interfaces

(a) $G_f=0.01 \text{ N/mm}$  
(b) $G_f=0.06 \text{ N/mm}$

Fig. 38. Crack surfaces with different cohesive energy of mortar-aggregate interfaces

It can be seen from Fig. 39, that the cohesive energy of aggregate-aggregate interfaces has little effect on the simulated stress-displacement curves. The crack paths, shown in Fig. 40, also have little dependence on the cohesive energy of aggregate-aggregate interfaces.

Fig. 39. Effect of cohesive energy for aggregate-aggregate interfaces
Fig. 40. Crack surfaces with different cohesive energy of aggregate-aggregate interfaces

The results shown in Fig. 41 indicate that the cohesive energy of mortar-mortar interfaces has a pronounced effect on shape of softening branch and a slight effect on peak stress. The stress in the post-peak range diminishes at a lower rate when the cohesive energy increases, which leads to a larger critical separation displacement. This suggests that the increase of cohesive energy for mortar-mortar interfaces result in a softer response of concrete samples under tension. Fig. 42 also shows that the crack paths are dependent on the cohesive energy of mortar-mortar interfaces.

![Graph showing the effect of cohesive energy on mean stress and displacement](image)

**Fig. 41. Effect of cohesive energy of mortar-mortar interfaces**

(a) $G_f=0.03$ N/mm  
(b) $G_f=0.06$ N/mm

![Graph showing crack surfaces with different cohesive energy](image)

**Fig. 42. Crack surfaces with different cohesive energy of mortar-mortar interfaces**

The effects of meso-scale material parameters, critical tensile stress and cohesive energy of meso-structure constituents, are logical and explain the variability in tensile...
strength and failure energy density (toughness) which is observed experimentally using variable mortar and aggregates.

5 Conclusions

Effective and efficient algorithms for generating three-dimensional meso-structures and corresponding finite element models with cohesive elements are developed. Meso-structures of concrete contain spherical, ellipsoidal or polyhedral aggregates, and spherical or ellipsoidal voids, dispersed in mortar, with intra-phase (aggregate/aggregate and mortar/mortar) and inter-phase (aggregate/mortar) cohesive elements. Monte Carlo approach is proposed for investigating the effects of 3D scaling, aggregate and void content, aggregate and void shape, and cohesive properties on longer-scale mechanical response. Core of the approach is statistical analysis of responses of 50 model realisations with given meso-structure parameters.

1. Mechanical response and crack propagation in concrete are affected strongly by the meso-structure: load carrying capacity decreases with increasing aggregate or void content and increasing aggregate roughness; Pre-peak response and peak stress are relatively insensitive to the aggregate and void spatial distribution; Post-peak softening response is sensitive to the spatial distribution of aggregates and voids;

2. Two macro-crack (failure) patterns are observed in concrete under uniaxial tension regardless of the shape of aggregate and void: Type I micro-cracks coalesce into one macro-crack propagating to failure. The result is rapid softening response and smaller failure energy density (apparent toughness of representative volume); Type II micro-cracks coalesce into two or more macro-cracks propagating concurrently to failure. The result is slower softening response and larger failure energy density (apparent toughness);

3. Compared to 2D modelling, the 3D modelling demonstrates: a larger mean peak stress and a smaller standard deviation in the pre-peak response, attributed to more uniformly distributed micro-cracks within the volume; A larger standard deviation in the post-peak response, attributed to the larger number of possibilities for micro-crack coalescence under the constraint of randomly distributed features;

4. The cohesive properties of concrete constituents affect strongly the macroscopic mechanical response and the cracking patterns: critical tensile stress of constituents has direct effect on the peak stress and differences between constituents’ strengths change the patterns of micro-crack coalescence and macro-crack
propagation; cohesive energy has little effect on the pre-peak behaviour, but affects strongly the softening behaviour and crack paths of concrete under tension.

It is acknowledged that all conclusions of this work are derived from meso-scale models of concrete subjected to uniaxial tension. The selection of simple zero-thickness cohesive elements with uncoupled tensile and shear responses has been dictated by this simple loading scenario. Development of advanced cohesive elements, specifically for coupling compressive and shear responses for simulations under more complex loading conditions, is a subject of ongoing research.

Acknowledgements

Wang acknowledges the support of the Faculty of Engineering and Physical Sciences via Dean’s Scholarship Programme at University of Manchester. Zhang and Jivkov acknowledge the support of EPSRC via Grant EP/J019763/1, “QUBE: Quasi-Brittle fracture: a 3D experimentally-validated approach”. The support of IT Services for the use of the Computational Shared Facility (CSF) at The University of Manchester is also gratefully acknowledged.

References


Appendix: Generation of individual random sphere, ellipsoid and convex polyhedron

A1 Sphere

A Cartesian $X$-$Y$-$Z$ coordinate system is used in generating concrete models. During the placing process, consider the standard equation of sphere:

$$(x-x_0)^2 + (y-y_0)^2 + (z-z_0)^2 \leq r^2$$  \hspace{1cm} (A.1)

where $x$, $y$, $z$ are the coordinates within the sphere, $x_0$, $y_0$, $z_0$ are the coordinates of centre of the sphere; $r$ is the radius of the sphere.

A2 Ellipsoid

An individual random ellipsoid can be generated by following three steps.

A2.1 A random size ellipsoid at original point

Considering the standard equation of ellipsoid at the original point:

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} \leq 1$$

$$a = r_0 + \eta \times (r_1 - r_0)$$ \hspace{1cm} (A.2)

$$b = \zeta a$$

$$c = \xi a$$

where $r_0$ and $r_1$ are the minimum and maximum radius in the size distribution, $\zeta$ and $\xi$ are random numbers within the aspect ratio range; $\eta$ is a random number uniformly distributed between 0 and 1.

An ellipsoid with random size at the original point in 3D space can then be described as
where \( a, b, c \) are the length of three semi-principal axes, \( X_{1}^{T} = \{x_{i}, y_{i}, z_{i}, 1\}^{T} \) is the homogeneous coordinates of any point on the ellipsoid surface.

**A2.2 Random rotation**

Any orientation can be achieved by composing three elemental rotations, starting from a known standard orientation. Equivalently, any rotation matrix \( R \) can be decomposed as a product of three elemental rotation matrices.

\[
R = Z^{1}(\alpha)X^{2}(\beta)Z^{3}(\gamma)
\]

(A.4)

\[
Z^{1}(\alpha) = \begin{bmatrix}
\cos(\alpha) & -\sin(\alpha) & 0 & 0 \\
\sin(\alpha) & \cos(\alpha) & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{bmatrix}
\]

(A.5)

\[
X^{2}(\beta) = \begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & \cos(\beta) & -\sin(\beta) & 0 \\
0 & \sin(\beta) & \cos(\beta) & 0 \\
0 & 0 & 0 & 1
\end{bmatrix}
\]

(A.6)

\[
Z^{3}(\gamma) = \begin{bmatrix}
\cos(\gamma) & -\sin(\gamma) & 0 & 0 \\
\sin(\gamma) & \cos(\gamma) & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{bmatrix}
\]

(A.7)

where, \( Z^{1}(\alpha), X^{2}(\beta), Z^{3}(\gamma) \) are the matrices representing the elemental sequential rotations about axes \( Z, X, Z \) of the fixed frame, (e.g., \( Z^{1}(\alpha) \) represents a rotation about \( Z \) axis by an angle \( \alpha \), \( X^{2}(\beta) \) represents a rotation about \( X \) axis by an angle \( \beta \), \( Z^{3}(\gamma) \) represents a rotation about \( Z \) axis by an angle \( \gamma \)). It should be noted that the final rotation could only be achieved with the specific sequence of rotations.

Then the coordinates of any points on the ellipsoid can be obtained as:

\[
X_{2} = RX_{1}
\]

(A.8)

**A2.3 Translation to a random position \((x_{0}, y_{0}, z_{0})\)**

The random ellipsoid can be translated to a random position \((x_{0}, y_{0}, z_{0})\) after random rotations, the coordinates on the ellipsoid are given by:
where $x_0, y_0, z_0$ are the coordinates of the center of the ellipsoid.

By substituting Equation (A.9) into Equation (A.8), and then into Equation (A4), a general equation of ellipsoid can be obtained as:

$$ F(x, y, z) = Ax^2 + By^2 + Cz^2 + Dxy + Exz + Fyz + Gx + Hy + Iz + J \leq 0 $$

(A.10)

Fig. A1 shows a few examples of numerical ellipsoids with different random numbers $(a, b, c, \alpha, \beta, \gamma)$.

(a) $a=6.3, b=4.2, c=4.2, \alpha = 344.8^\circ, \beta = 87.4^\circ, \gamma = 288.2^\circ$

(b) $a=5.4, b=4.7, c=4.8, \alpha = 67.3^\circ, \beta = 88.2^\circ, \gamma = 160.5^\circ$

(c) $a=5.1, b=2.2, c=3.2, \alpha = 182.2^\circ, \beta = 125.9^\circ, \gamma = 320.9^\circ$

Fig. A1. Configuration of random ellipsoids

A3 Polyhedron

The polyhedrons can be generated by randomly picking the nodes on the spheres using spherical coordinate system as follows,

$$ \bar{x}_i = r' \cos(\theta) \sin(\phi) + x_0 $$

$$ \bar{y}_i = r' \sin(\theta) \cos(\phi) + y_0 $$

$$ \bar{z}_i = r' \cos(\phi) + z_0 $$

(A.11)

where $\bar{x}_i, \bar{y}_i, \bar{z}_i$ are the coordinates of the $i^{th}$ vertex of the polyhedron. $x_0, y_0, z_0$ are the coordinates of the center of the sphere, $r'$ is the radius of the sphere.

$$ r' = r_0 + \eta \times (r_1 - r_0) $$

$$ \theta = \zeta \times 2\pi $$

$$ \phi = \xi \times \pi $$

(A.12)

where $\theta$ is the polar angle measured from a fixed zenith direction, $\phi$ is the azimuth angle of its orthogonal projection on a reference plane that passes through the origin and is orthogonal to the zenith, measured from a fixed reference direction on that plane. $r_0$ and $r_1$ are the minimum and maximum radius in the size distribution. $\eta, \zeta, \xi$ are independent random numbers uniformly distributed between 0 and 1.
In order to make sure the randomness of generated polyhedrons, the number of vertexes of polyhedron is determined as uniformly distributed from $N_{\text{min}}$ to $N_{\text{max}}$ as

$$N = N_{\text{min}} + \eta \times (N_{\text{max}} - N_{\text{min}})$$  \hspace{0.5cm} (A.13)

where $\eta$ is a random number uniformly distributed between 0 and 1.

The polyhedrons are generated by linking the nearest three vertexes to an area, and then make all the areas connected to a volume. To get a better quality mesh for finite element modelling, a minimum distance limitation between every two vertexes is set to $0.5r'$. Fig. A2 shows a few examples of numerical polyhedrons with different random numbers.

Fig. A2. Configuration of random polyhedrons
Combined Numerical-statistical Analyses of Damage and Failure of 2D and 3D Mesoscale Heterogeneous Concrete

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Published in Mathematical Problems in Engineering. 2015; 501:702563.

6.1 Statement of own contributions in joint authorship

Main research technology development;
Preparation of tables and figures, and writing of the manuscript;
Finite element modelling by ABAQUS;
Data processing and analysis;
Interpretation of results.

6.2 Paper in the research context

This paper compares the 2D Monte Carlo simulations in Chapter 3 and 3D numerical work in Chapter 5 on geometrical representation of heterogeneous concrete, load-carrying capacities, toughness, statistical distribution of specimen strength, and crack patterns, etc.

The third dimension is demonstrated to have a pronounced influence on both macroscopic mechanical properties and crack patterns in tension; compared to 2D modelling, 3D modelling demonstrates a larger mean peak stress and a smaller standard deviation in the pre-peak response, attributed to more uniformly distributed micro-cracks within the specimen; a larger standard deviation/coefficient of variation of stress in the post-peak response is attributed to the larger number of possibilities for micro-crack coalescence under the constraint of randomly distributed features.

This Chapter is an exact copy of the journal paper referred to above.
(See Paper IV as follows)
Combined Numerical-Statistical Analyses of Damage and Failure of 2D and 3D Mesoscale Heterogeneous Concrete

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Generation and packing algorithms are developed to create models of mesoscale heterogeneous concrete with randomly distributed elliptical/polygonal aggregates and circular/elliptical voids in two dimensions (2D) or ellipsoidal/polyhedral aggregates and spherical/ellipsoidal voids in three dimensions (3D). The generation process is based on the Monte Carlo simulation method wherein the aggregates and voids are generated from prescribed distributions of their size, shape, and volume fraction. A combined numerical-statistical method is proposed to investigate damage and failure of mesoscale heterogeneous concrete: the geometrical models are first generated and meshed automatically, simulated by using cohesive zone model, and then results are statistically analysed. Zero-thickness cohesive elements with different traction-separation laws within the mortar, within the aggregates, and at the interfaces between these phases are preinserted inside solid element meshes to represent potential cracks. The proposed methodology provides an effective and efficient tool for damage and failure analysis of mesoscale heterogeneous concrete, and a comprehensive study was conducted for both 2D and 3D concrete in this paper.

1. Introduction

Concrete is the most widely used construction material in the world due to its good strength and durability relative to its cost. Numerical simulations coupled with theory and experiment are considered to be an important tool for examining the mechanical behaviour through computational materials science. Wittmann [1] proposed three levels of observation: microlevel (10^{-6} m), mesolevel (10^{-3} m), and macrolevel (10^0 m). The microlevel represents the most basic level, in which the internal structure of cement paste is considered and where physical and chemical forces dominate. In the mesolevel, concrete is usually represented as a material made up of coarse aggregates, mortar with fine aggregates and cement paste embedded inside, and interfaces between coarse aggregates and mortar. At the macroscale, concrete is treated as a homogenous and continuous material in which the internal structure is not considered [2]. As concrete is generally used in large-sized structures and its dependence of mechanical behaviours on mesostructures is significant, mesoscale modelling of concrete becomes essential and was investigated in this study.

An extensive literature review recently carried out by Wang et al. [3] shows that numerical image processing technique and parameterization modelling technique are two main approaches to generate mesostructure models of concrete. Although the mesh generated from images is closest to nature, it is presently very costly and time consuming to generate sufficient scanned images and convert them to mesh for meaningful statistical analyses (e.g., [4–6]). In the parameterization modelling technique, both direct (e.g., [3, 7–9]) and indirect approaches (e.g., [10–13]) to characterize material random heterogeneity have been used. The indirect approach is able to generate a large number of samples with ease but the key multiphasic parameters which could significantly influence the mechanical behaviour cannot be considered. The direct approach can take into account most of the key parameters such as shape, size, gradation and spatial distribution of voids and aggregates, phase volume fractions, and aggregate-mortar interfaces. So among all the approaches, it seems that the direct approach is particularly suitable for statistical analysis of concrete samples and was used in this study.
Identification and generation of unit cell geometry are a vital step in the mesoscale analysis of concrete. Both shape and size of aggregates have significant influences on the stress distribution, crack initiation, and damage accumulation up to the macroscopic failure within the concrete material [16]. Most of the existing algorithms for mesostructure generation of concrete only consider random aggregates but neglect voids [2, 7, 17–19]. However, the X-ray CT images [4, 14, 20] clearly show that voids exist in concrete at this scale and have severely adverse effects on the specimen strength [3, 9]. So automatic generation of morphological details of materials with randomly distributed different shape of aggregates and voids poses new challenges. In this paper, a computationally efficient and versatile in-house program of heterogeneous material generator (HMG) has been developed considering both 2D and 3D random aggregates and voids based on the prescribed parameters.

Several numerical models for crack propagation at mesoscopic level have been used to study the heterogeneity of concrete. Continuum based finite element models are the main approaches employed in the literature [21–24], primarily based on cohesive zone model [25]. Other alternative approaches have also been developed, such as discrete element model (DEM) [26] and lattice model [11, 12]. The biggest disadvantage of DEM and lattice model is the difficulty in determining the equivalent model parameters, which is relatively straightforward for continuum based finite element models [27]. The numerical model used in this work for crack propagation at mesoscopic level is based on the cohesive zone model [3]. It is becoming more and more popular in modelling crack propagation due to its simple formation and easy implementation in the form of cohesive interface elements (CIEs).

With the preprocessing functionality in ANSYS [29] and explicit solver in ABAQUS [30], nonlinear modelling of multiple crack propagation with a considerable number of concrete samples has been performed by high performance computing in this study. Statistically, analysis of mechanical behaviour of both 2D and 3D specimens has been conducted using the combined numerical-statistical method, leading to valuable statistical results that may help improve designs of concrete materials.

### 2. 2D and 3D Heterogeneous Concrete

#### 2.1. Aggregate and Void Size Distribution

The size distribution of aggregates in concrete is often described by the Fuller curve [16], which is discretised into a certain number of segments. The aggregate size distributions found in Hirsch [28] and summarised in Table 1 are used in this study. In this study, concrete is treated as a material consisting of coarse aggregates, mortar incorporating fine aggregates dissolved in it, voids, and interfaces between aggregates and mortar. Here only coarse aggregates are explicitly modelled as mesoscale features. For normal strength concrete cast with a mould in the laboratory, coarse aggregates usually represent 30–50% of the concrete volume.

From X-ray CT images, it was found that gravel aggregates have circular/elliptical shapes in 2D and spheroidal/ellipsoidal shapes in 3D, while crushed aggregates have polygonal shapes in 2D and polyhedral shapes in 3D [14]. A number of voids can be clearly observed in concrete at mesoscale from CT images (see Figure 1). Therefore, voids with size ranging from 2 to 4 mm as presented in [31] are included in the mesostructure of concrete in this study. Coarse aggregates are considered to have elliptical/polygonal shapes in 2D and ellipsoidal/polyhedral shapes in 3D.

<table>
<thead>
<tr>
<th>Sieve size (mm)</th>
<th>Total percentage retained (%)</th>
<th>Total percentage passing (%)</th>
</tr>
</thead>
<tbody>
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<td>12.70</td>
<td>0</td>
<td>100</td>
</tr>
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<td>9.50</td>
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<td>4.75</td>
<td>90</td>
<td>10</td>
</tr>
<tr>
<td>2.36</td>
<td>98.6</td>
<td>1.4</td>
</tr>
</tbody>
</table>

![Figure 1: Tomographic cross-sectional view of three concretes varying by coarse aggregate shape (after [14]).](image-url)
2.2 Specimen Generation. The basic idea is to create the aggregates and voids in the concrete in a repeated manner, until the target area/volume is filled with aggregates and voids. The generation starts with the information input process and is followed by taking and placing voids within size range; the aggregates within the grading segments are produced last. The “input” process reads the controlling parameters for generating a heterogeneous concrete; the “taking” process generates an individual void or aggregate in accordance with the random size and shape descriptions. The “placing” process positions the aggregates and voids into the predefined area/volume in a random manner, subject to the prescribed physical constraints. There are three physical conditions to be satisfied simultaneously: (1) the whole inclusion (void or aggregate) must be within the concrete, (2) there is no overlapping of inclusions, and (3) there is no intersection between any two inclusions. A three-level hierarchical method is proposed to reduce the computational cost and is outlined in Figure 2. The procedure was programmed using MATLAB [32] in this study, and the detailed algorithms and procedure in generating mesostructures can be found in our previous work [3, 33].

2.3 Mesostructure Models. Elliptical aggregates and circular/elliptical voids in 2D or ellipsoidal aggregates and spherical/ellipsoidal voids in 3D were used for concrete with gravel aggregates. A series of concrete samples with dimensions of 50 mm × 50 mm in 2D and 50 mm × 50 mm × 50 mm in 3D are generated. Figure 3 shows the numerically generated models with gravel aggregates (aggregates in green and voids in red). Aggregate gradation in Table 1, aggregate volume fraction \(P_{\text{agg}} = 30\%\), void content \(P_{\text{void}} = 2\%\), aspect ratios for elliptical/ellipsoidal aggregates and voids (the ratio of the major axis to the minor axis) \(R_1 = R_2 = [1, 2]\), minimum space between the edge of an aggregate and the boundary of the concrete specimen \(y_1 = 0.2\) mm, and minimum gap width between any two aggregates \(y_2 = 0.2\) mm are adopted here [31].

Polygonal aggregates and circular/elliptical voids in 2D or polyhedral aggregates and spherical/ellipsoidal voids in 3D are considered for concrete with crushed aggregates. A series of concrete samples with the same dimensions as the previous gravel aggregate samples are generated. Figure 4 shows the numerically generated models with crushed aggregates. The minimum and maximum edges of the polygons/polyhedrons are set to \(N_{\text{min}} = 8\), \(N_{\text{max}} = 16\). All the other parameters are the same as the values used for gravel aggregates.
3. Combined Numerical-Statistical Method

3.1. Description of the Method. A combined numerical-statistical method is proposed in this paper to study the material behaviour of concrete in a statistical sense. The detailed procedure is as follows:

1. Generate a model with prescribed variables, for example, sample size, aggregate volume fraction, void content, and aggregate shape.

2. Perform a finite element simulation of the sample for given boundary conditions.

3. Compute the mean value, standard deviation, and coefficient of variation (CoV) of effective property for the considered sample size.

4. Repeat steps (1) to (3) for sufficient number of random samples to meet the required precision, and conduct statistical analysis.

This procedure is automated by running a batch file in this study.

Results from all realisations are evaluated statistically. The standard deviation $s$ within a series of $n$ samples is given by

$$s^2 = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x})^2,\quad (1)$$

where $\bar{x} = (1/n) \sum_{i=1}^{n} x_i$ is the series average result and $x_i$ is the result from sample $i$.

To compare results obtained with different sample sizes quantitatively, we use the coefficient of variation given by

$$\varepsilon = \frac{s}{\bar{x}}.\quad (2)$$

This expresses the fluctuation of measured property relative to its average value.

3.2. Cohesive Zone Model in ABAQUS. The cohesive zone model developed by Barenblatt [34, 35] and Dugdale [36] enables the simulation of the energy dissipation process in the fracture process zone (FPZ) during fracture, as illustrated in Figure 5. A bilinear cohesive crack model is used here to predict discrete crack propagation in concrete specimens under tension loading. A linear ascending branch is added in the softening curve to model the initially uncracked material.

The separation displacement is difficult to derive from experiments, so cohesive fracture energy and cohesive strength are usually used. Among them, only two parameters are independent, and the fracture energy can be obtained as

$$G = \int_{\delta_f}^{t_f} t(\delta) d\delta = \frac{1}{2} t_0 \delta_f,\quad (3)$$

where $G$ is the cohesive fracture energy, $t_0$ is the cohesive strength, and $\delta_f$ is the separation displacement.

In the 3D cohesive zone model, it is assumed that there exist a normal traction $t_n$ and two tangential tractions (shear cohesion) $t_t$ and $t_t$ across the crack surfaces, through mechanisms such as material bonding, aggregate interlocking, and surface friction in the fracture process zone. Figures 6(a) and 6(b) illustrate typical linear softening curves for $t_n - \delta_n$ and $t_t(t_t) - \delta_t(\delta_t)$, where $\delta_n$ and $\delta_t(\delta_t)$ are the critical relative displacements when the tractions diminish for normal traction and tangential traction components, respectively. The unloading paths are also indicated.

It is worth noting that the initial tensile stiffness $k_{n0}$ should be high enough to ensure displacement continuity across the cohesive interfaces before the tensile strength $t_{n0}$ is reached, but not too high to cause numerical instability due to ill-conditioned global stiffness matrix. Reasonable initial shear stiffness, $k_{t0}$ and $k_{t0}$, is also needed before the shear strength, $t_{t0}$ or $t_{t0}$, is reached. The effects of initial stiffness on computational results have been investigated previously [37, 38]. The following relation is suggested in [38] as a guideline for initial stiffness selection:

$$k_{n0} = k_{t0} = k_{t0} = \frac{c(1-v)}{b(1+v)(1-2v)}E,\quad (4)$$

where $E$ and $v$ are Young’s modulus and Poisson’s ratio, $b$ is the characteristic size of elements, and $c$ is taken as 10-100 from the experience in [38].

The areas under the curves in Figures 6(a) and 6(b) (calculated by (3)) represent the normal fracture energy
$G_{nf}$ and twice the tangential fracture energy, $G_{sf}$ and $G_{tf}$, respectively:

$$G_{nf} = \int_0^{\delta_{nf}} t_n (\delta_n) \, d\delta_n = \frac{1}{2} t_{n0} \delta_{nf},$$

$$G_{sf} = \int_0^{\delta_{sf}} t_s (\delta_s) \, d\delta_s = \frac{1}{2} t_{s0} \delta_{sf},$$

$$G_{tf} = \int_0^{\delta_{tf}} t_t (\delta_t) \, d\delta_t = \frac{1}{2} t_{t0} \delta_{tf}. \quad (5)$$

Cohesive elements in ABAQUS based on the cohesive zone model are used here. The damage is characterised by a scalar index $D$ representing the overall damage of the crack caused by all physical mechanisms. The effective relative displacements $\delta_m$ combining the effects of $\delta_n$, $\delta_s$, and $\delta_t$ can be obtained as

$$\delta_m = \sqrt{\langle \delta_n \rangle^2 + \delta_s^2 + \delta_t^2}, \quad (6)$$

where $\langle \rangle$ is the Macaulay bracket and

$$\langle \delta_n \rangle = \begin{cases} \delta_n, & \delta_n \geq 0 \text{ (tension)} \\ 0, & \delta_n < 0 \text{ (compression)}. \end{cases} \quad (7)$$

The damage evolution law is given by

$$D = \frac{\delta_{mf} (\delta_{m,\text{max}} - \delta_{m0})}{\delta_{m,\text{max}} (\delta_{mf} - \delta_{m0})}, \quad (8)$$

where $\delta_{m,\text{max}}$ is the maximum effective relative displacement attained during the loading history, $\delta_{m0}$ and $\delta_{mf}$ are effective
relative displacements at damage initiation and complete failure, respectively. It is obvious that the damage variable \( D \) evolves monotonically from 0 to 1 upon further loading after the initiation of damage.

The damage initiation and evolution will degrade the unloading and reloading stiffness coefficients \( k_n \), \( k_s \), and \( k_t \), which can be calculated as

\[
\begin{align*}
    k_n &= (1 - D) k_{n0}, \\
    k_s &= (1 - D) k_{s0}, \\
    k_t &= (1 - D) k_{t0}.
\end{align*}
\]

(9)

The tractions are also affected by the damage according to

\[
\begin{align*}
    t_n &= \begin{cases} (1 - D) \bar{t}_n, & \bar{t}_n \geq 0 \\
                     \bar{t}_n, & \bar{t}_n < 0 \end{cases} \\
    t_s &= (1 - D) \bar{t}_s, \\
    t_t &= (1 - D) \bar{t}_t,
\end{align*}
\]

(10)

where \( \bar{t}_n \) and \( \bar{t}_s \) are the traction components predicted by the elastic traction-displacement behaviour for the current separation without damage.

In this study, damage in the cohesive zone model is assumed to initiate when a quadratic interaction function involving the nominal stress ratios reaches a value of one

\[
\left( \frac{t_n}{t_{n0}} \right)^2 + \left( \frac{t_s}{t_{s0}} \right)^2 + \left( \frac{t_t}{t_{t0}} \right)^2 = 1.
\]

(11)

The material properties, such as density, Young’s modulus, Poisson’s ratio, tensile strength, and fracture energy, are set for continuum elements of aggregates and mortar, three different interface cohesive elements. The material heterogeneity is investigated by considering different phases in the concrete specimen with corresponding material properties.

In the fracture process zone for a 2D case, tractions exist in the normal direction \( t_n \) and shear direction \( t_s \) across the crack interface, and the corresponding relative displacements are \( \delta_n \) and \( \delta_s \). So the 2D constitutive law could be easily deduced from 3D characterization described above by taking one of the shear tractions and displacements out.

3.3. Cohesive Interface Elements Insertion. In this study, all finite element meshing is performed with the preprocessing functionality in commercial FE package ANSYS [29]. To mesh the mesoscopic structure of concrete, different material parts (mortar and aggregates) should maintain continuity on their surfaces. Hence, the finite element boundaries are coincident with material surfaces and there are no material discontinuities within the elements. The mortar and aggregates are meshed with triangular elements (plain stress) in 2D and hexahedral elements in 3D so that more realistic crack paths can be obtained. The specially developed ANSYS parametric design language (APDL) programs in combination with the ANSYS batch processing provide a powerful tool of automatic

mesh generation for a large number of samples required for statistical analysis. Following the meshing procedure, the generated mesh will automatically have shared nodes at the interfaces between two elements. If the interfaces surrounding the elements are to be modelled explicitly as potential microcrack sources, a duplicate set of nodes will be required at the interface locations. Here 4-node or 6-node zero in-plane thickness CIEs are preinserted into the existing element interfaces in 2D or 3D. This is conducted by a purpose written and flexible in-house computer program cohesive interface elements insertion (CIEIN). Three sets of CIEs with different traction-separation softening laws are inserted (see Figure 7), namely, CIE-AGG inside the aggregates (grey in Figures 7(b) and 7(d)), CIE-MOR inside the mortar (green in Figures 7(b) and 7(d)), and CIE-INT on the aggregate-mortar interfaces (yellow in Figures 7(b) and 7(d)). The element and node numbers are denoted by \( E \) and \( N \), respectively. The detailed numbering of elements and nodes in the initial mesh and the mesh with inserted cohesive elements shows the insertion procedure with the new nodes generated at the same positions and CIEs between the continuum elements.

4. Numerical Simulation and Results

4.1. Description of the Numerical Model. 2D concrete specimens with elliptical aggregates and circular voids and 3D specimens with ellipsoidal aggregates and spherical voids (\( P_{\text{agg}} = 30\% \), \( P_{\text{void}} = 2\% \), \( R_1 = R_2 = [1, 2] \), \( y_1 = y_2 = 0.2 \text{ mm} \)) were modelled, loaded under uniaxial tension. 25 mm × 25 mm concrete square in 2D and 25 mm × 25 mm × 25 mm concrete cubic in 3D are used here. All the other mesoscale parameters were fixed to be the same for 2D and 3D models. Figure 8 shows the geometry, boundary, and loading conditions of the numerical model. Horizontal displacements were prescribed to all nodes on the left and right surfaces of the specimen, with a value equal to zero for the left surface, and a uniformly distributed displacement on the right surface. Vertical displacements for the same nodes are left free, except for the nodes at the lower left corner of the specimen, which are fixed to prevent rigid body translation. A displacement controlled loading scheme was used and all the analyses were ended at a displacement \( d = 0.1 \text{ mm} \) and loading time \( t = 0.005 \text{ s} \) [3]. Considering the balance between accuracy and efficiency, the element length \( 1 \text{ mm} \) was used for all the meshes in this study [3].

Generally, aggregates have much higher strength than mortar and interfaces in normal concrete. In this section, no cracks are allowed to initiate inside the aggregates by assuming elastic behaviour without damage in CIE-AGG. The linear tension/shear softening laws described above were used to model CIEs with quadratic nominal stress initiation criterion and linear damage evolution criterion. Similar material properties extracted from [39] were used in this study, which are listed in Table 2. The fracture properties related to the shear behaviour were assumed to be the same as the normal ones due to the lack of experimental data. Both initial tensile and shear stiffness for all the cohesive elements were set to \( 10^6 \text{ MPa/mm} \) after trial and error.
Figure 7: Inserting different cohesive elements to the initial mesh.

Table 2: Material properties.

<table>
<thead>
<tr>
<th></th>
<th>Young’s modulus E (MPa)</th>
<th>Poisson’s ratio $\nu$</th>
<th>Density $\rho$ ($10^9$ tonne/mm$^3$)</th>
<th>Elastic stiffness $k_n$ (MPa/mm)</th>
<th>Cohesive strength $t_n$ (MPa)</th>
<th>Fracture energy $G_F$ (N/mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aggregate</td>
<td>70000</td>
<td>0.2</td>
<td>2.8</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Mortar</td>
<td>25000</td>
<td>0.2</td>
<td>2.0</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>CIE-AGG</td>
<td>—</td>
<td>—</td>
<td>2.8</td>
<td>—</td>
<td>10$^6$</td>
<td>—</td>
</tr>
<tr>
<td>CIE-MOR</td>
<td>—</td>
<td>—</td>
<td>2.5</td>
<td>10$^6$</td>
<td>4</td>
<td>0.06</td>
</tr>
<tr>
<td>CIE-INT</td>
<td>—</td>
<td>—</td>
<td>2.0</td>
<td>10$^6$</td>
<td>2</td>
<td>0.03</td>
</tr>
</tbody>
</table>
ABAQUS/explicit with small time increments (typically $\Delta t = 3 \times 10^{-8}$ s) was utilised to solve the highly nonlinear equation systems by the high performance computing (HPC) cluster at the University of Manchester computational shared facility (CSF). A typical run of simulations with 50 samples in this study takes about 6 hours by parallel computation with 32 CPUs.

4.2. Tensile Behaviour. Due to the statistical nature of mesostructure models, an extensive series of numerical simulations would be necessary to capture the range of behaviours. Fifty random samples were modelled in this study to ensure that the results are statistically converged.

In Figure 9, resulting mean stress-displacement and toughness-displacement curves, together with the variation range for both 2D and 3D, are depicted. It can be seen that the predicted stress-displacement curves are qualitatively similar with a clear peak and sharp initial postpeak drop followed by a long shallow tail. Numerical mean stress for every curve is obtained by summing the nodal reaction forces in the constraints and dividing by the specimen cross section area. The mean peak stress predicted by 2D
and 3D modelling is 2.65 MPa and 3.49 MPa, respectively, representing an increase of 24.1%. The mean toughness (energy absorbed per unit volume up to the break point, i.e., the area under the stress-strain curve up to the break point, measured in J/m$^3$) predicted in 2D and 3D modelling is 2.47 KJ/m$^3$ and 3.15 KJ/m$^3$, respectively, representing an increase of 21.6%; Figure 10 shows the standard deviation-displacement curves for both 2D and 3D modelling. The standard deviation of peak stress is 0.11 MPa and 0.05 MPa, respectively, representing a decrease of 54.5%. These increases in peak stress or decreases in standard deviation are due to the constraint effects in the thickness direction in 3D and the less smooth cracking surfaces from 3D modelling. However, the standard deviation of 3D modelling at softening range is larger than that in 2D modelling which indicates that 3D modelling is more complicated and dependent on different samples. This is due to the 3D heterogenous distribution of aggregates and voids. It is clear that the third dimension cannot be neglected due to the nature of fracture process. The importance of the thickness effect has also been pointed out experimentally by Van Mier and Schlangen [40].

The mean curve, mean value, and standard deviation of the stress and toughness shown in Figures 9 and 10 are extracted from the stress-displacement curves for 50 samples with different aggregate and void distribution. In order to evaluate the effect of sample number on simulation results as required for the proposed combined numerical-statistical method, two special loading points, namely, point A at peak stress and point B at displacement 0.03mm where largest standard deviation is observed (denoted in Figures 9(a) and 10), are investigated. The influence of sample number on the CoV of stress at points A and B is illustrated in Figure 11. It can be seen that 50 samples are enough to get convergent values of CoV of stress with a stable fluctuation. This is an indication that the combined numerical-statistical method with 50 random realisations offers a good balance between general applicability and testing of different samples. It can be observed that COV of peak stress for different void and aggregate distribution is low (4.2% for 2D modelling and 1.5% for 3D modelling), which demonstrates that the peak stress is relatively insensitive to the void and aggregate distribution. The high CoV of stress at point B further demonstrates the necessity to conduct a statistical analysis as the results vary greatly for different aggregate and void distribution in softening range.

Figure 11 shows the statistical distribution of peak stress, together with the probability density and the best fit Gaussian Probability Density Function (PDF). The probability density curve can be used to calculate structural reliability or failure reliability against given external loadings and material properties for structural design.

4.3. Crack Patterns. The complex mesoscale crack propagation is realistically simulated using the proposed method, and typical crack patterns for both 2D and 3D at failure are shown in Figure 13. To clearly visualise the fracture surfaces, models with damaged cohesive elements, models without cohesive elements, and failed interfaces only are used for 2D models (see Figures 13(a)–13(c)), and models with damaged cohesive elements, models without cohesive elements, and morphology of failed surface are used for 3D models (see Figures 13(d)–13(f)). The cracks shown in Figures 13(a), 13(c), and 13(d) are represented by red CIEs with damage index $D \geq 0.95$ ($D = 1$ means complete failure). A magnification factor of 20 and 200 was used for the deformed models with damaged CIEs and those without damaged CIEs, respectively. The noticeable difference of 2D and 3D modelling discussed above could also be summarized in that the 3D modeling predicts more realistic fracture surfaces in the thickness direction whereas 2D modeling only assumes plane fracture problems. This result confirms the importance of including the third dimension into the analysis.
Figure 12: Statistical distribution of peak stress from Monte Carlo simulation.

(a) 2D model with damaged CIEs
(b) 2D models without CIEs
(c) 2D models with failed interfaces
(d) 3D model with damaged CIEs
(e) 3D model without CIEs
(f) 3D morphology of failed surface

Figure 13: Failure of concrete under tension.
5. Conclusions

Models of numerical concrete with random mesostructures comprising elliptical/polygonal aggregates and circular/elliptical voids in 2D and ellipsoidal/polyhedral aggregates and spherical/ellipsoidal voids in 3D have been generated in this study. Numerical-statistical analysis was carried out using a cohesive zone model to simulate damage and failure of concrete. Crack patterns are realistically simulated using the technique of preembedding cohesive interface elements. The main conclusions, based on the results obtained from the statistical analysis under a uniaxial tension loading, are as follows: (1) statistical analysis is necessary in both 2D and 3D due to the high dependence of material behaviour on different aggregate and void spatial distribution; (2) the third dimension is demonstrated to have a pronounced influence on both macroscopic mechanical properties and crack patterns in tension; (3) compared to 2D modelling, 3D modelling demonstrates a larger mean peak stress and a smaller standard deviation in the prepeak response, attributed to more uniformly distributed microcracks within the specimen; a larger standard deviation/CoV of stress in the postpeak response is attributed to the larger number of possibilities for microcrack coalescence under the constraint of randomly distributed features. It has to be pointed out that the conclusions obtained are based on mesoscale modelling with specific specimen and aggregate size. The variation on resulting mechanical behaviour is also associated with the size of specimen and aggregates, and this phenomenon may not exist when specimen is large enough, for example, at the length scale of engineering structures.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

Acknowledgments

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References


CHAPTER SEVEN

3D Meso-structural Modelling of Concrete for Damage and Failure Analysis in Tension and Compression

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Submitted to Cement and concrete research.

7.1 Statement of own contributions of joint authorship

Main research idea development and technological planning;
Preparation of tables and figures, and writing of the manuscript;
In-house APDL and MATLAB programs development for pre-processing in 3D;
Finite element calculation by ABAQUS;
Python script writing for data processing;
Statistical analysis and result interpretation.

7.2 Paper in the research context

This paper presents an alternative computational technology for damage and failure analysis of heterogeneous quasi-brittle materials, applied to concrete. It is based on the numerically generated synthetic 3D meso-structures developed in Chapter 5, while non-zero thickness but very thin layers of ITZs are identified between aggregates and mortar. Unlike the studies carried out in Chapters 3, 4 and 5, the alternative scheme for identification of ITZs employs equivalent solid elements equipped with damage-plasticity constitutive laws is adopted. By using damage-plasticity constitutive laws to the solid elements of mortar and ITZs, the new scheme avoids the difficulties associated with typical cohesive zone models under compressive stress conditions. A 3D meso-structural modelling of concrete is performed in tension and compression in this paper to interpret the fundamental mechanisms of crack initiation and propagation. The aggregate and void distribution is demonstrated to have a pronounced influence on both the macroscopic stress-strain
behaviour and the crack patterns for compression and tension. The load-carrying capacity decreases as the void content increases in both compression and tension, and it is also found that void content has a large effect on the load-carrying capacity and final cracking patterns.

This Chapter is an exact copy of the journal paper referred to above.

(See Paper V as follows)
3D Meso-structural Modelling of Concrete for Damage and Failure Analysis in Tension and Compression

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Abstract: Damage and failure of concrete are analysed by synthetic meso-structures including four phases: aggregates, mortar, interfacial transaction zones (ITZs) and voids. Models generation is controlled by meso-structure characteristics: shape, size, volume fraction and spatial distribution of aggregates and voids. ITZs are represented by thin layers between mortar and aggregates. Aggregates are modelled with linear elastic, while mortar and ITZs with different continuum damage-plasticity behaviours.

Tensile and compressive behaviour of concrete, including nucleation, coalescence, and propagation of cracks, are studied. The stress-strain response and the damage to failure transition are found to be dependent strongly on the meso-structure, particularly the post peak softening. Void content, generally ignored in meso-structure models, is shown to affect significantly the concrete behaviour. Average deformation and failure behaviour from the simulations agrees very well with experimental tensile and compressive data. The methodology is applicable to a large class of composite materials with appropriate selection of phases’ properties.

Keywords: Concrete, Meso-structure, Interfacial transaction zone, Damage-plasticity, Random generation

1. Introduction

Concrete is a complex composite with sub-continuum structures at multiple length scales. The largest length-scale with observable heterogeneity is traditionally called the meso-scale. The meso-structure of concrete contains voids, aggregates, mortar, and interfaces between them. Being closest to the component scale, the meso-structure plays a critical role in the observable macroscopic behaviour of concrete [1].

In the multiphase composition of concrete, interfacial transaction zones (ITZs) are the very thin layers of material surrounding the aggregates [2]. It is well known that ITZs play a very important role in concrete fracture behaviour, and are considered as the weakest link in a concrete composite. The thickness of ITZs is typically in the

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range of 10-30 μm [3]. Some previous works did not consider ITZs as a separate phase and assumed perfect bonding between aggregates and mortar [4, 5]. This appears to be an oversimplification due to different mechanical behaviour of ITZs from the mortar. Although this has not been fully characterised yet experimentally, due to the complexity of their microstructures and the constraints of existing measurement techniques [6, 7], there are indications that both the compressive and tensile strength of the ITZs are 50% to 100% of the mortar [8-10]. These differences can be accounted for by modelling ITZs with either zero-thickness cohesive interface elements [1, 10], or with standard solid elements of prescribed thickness [2, 6]. An exact representation of the real ITZ thickness with solid elements at the meso-scale would lead to too fine meshes and challenging analysis. Therefore, the ITZ thickness was assumed to be between 0.1 mm and 1 mm in most of previous numerical studies [2, 6, 9, 11]. Kim and Abu Al-Rub [6] found that the change of ITZ thickness from 0.1 mm to 0.8 mm had little effect on the post-peak behaviour of concrete. Based on these past results, the present study uses 0.3 mm thick solid elements to represent ITZs as a separate phase with tensile and compressive strength approximately 75% of the mortar’s as suggested in Lu and Tu [12].

A number of meso-scale models, considering the meso-structure and the local failure mechanisms in concrete, have been proposed in the last few decades, aiming at better understanding of structures on longer-scale response of concrete [13, 14]. Continuum based finite element models are the main approaches employed in the literature [15, 16], mostly based on the damage-plasticity model [6, 17] and the cohesive zone model [18-21]. The damage-plasticity model provides a general capability for modelling concrete and other quasi-brittle materials by assuming damaged elasticity in combination with tensile and compressive plasticity. In the cohesive zone models, cohesive interface elements are pre- or dynamically inserted into the finite element mesh so that realistic crack patterns can be simulated [10]. Other alternative approaches have also been developed, such as discrete element models [22] and lattice models [23]. One challenge with these proposals is the calculation of equivalent model parameters, i.e. force-displacement relations need to be calibrated by macroscopic stress-strain data. This is avoided when using continuum based FE model. The nonlinear finite element simulations conducted in this work for damage and failure analysis of concrete are based on the damage-plasticity model [24]. Aggregates are assumed to be elastic, and different softening constitutive laws for
mortar and ITZs are specified. This allows potential cracks to nucleate and propagate across the mortar and along the ITZs.

The generation of actual 3D model with distributed random aggregates is not a trivial task, and most of the meso-scale modelling of concrete has been conducted with 2D samples. Further, the majority of past works treat concrete as a two phase (mortar, aggregates) or three phase (mortar, aggregates and interfaces) material at the meso-scale [25-27]. However, X-ray Computed Tomography images of concrete show clearly that voids exist in the concrete at this scale [28]. Therefore, volume fraction, size, gradation, spatial distribution of aggregates and voids should be considered as important for adequate meso-structure description. Several methods been used for generation of 3D concrete meso-structures: Voronoi tessellation [29], lattice model [30], and Monte Carlo random sampling [31], etc. In these models, however, volume fraction, size distribution and shape of aggregates are not explicitly considered. In this paper, 3D heterogeneous concrete specimens with randomly distributed spherical, ellipsoidal, polyhedral aggregates and spherical voids are generated by a three-level hierarchical method [10, 32], where aggregates and voids obey prescribed distributions of size, shape and volume fraction.

The aim of this study is to contribute to the design of superior fracture resistant concrete, by further clarifying the effects of meso-structure characteristics on its macroscopic behaviour in engineering structures. Effective and efficient simulation of 3D damage evolution and failure of concrete at the meso-scale is now possible, due to the recent advances in understanding the mechanical behaviour of concrete’s different phases and the developments in computational capability. Building on the recent advances, the work formulates 3D meso-scale models, reports and analyses the outcomes of the simulations. The report is organized as follows: Section 2 describes the meso-structure geometric model and mesh generation; Section 3 presents the numerical framework of the damage-plasticity model used; Section 4 defines the finite element models analysed; Section 5 reports and discusses the main simulation results on compression and tension; Section 6 summarises the conclusions from the work.

2. Meso-structure models and mesh generation

2.1 Meso-scale model of concrete

An extensive investigation recently carried out by Wang et al. [32] shows that gravel aggregates have spherical/ellipsoidal shapes, while crushed aggregates have
polyhedral shapes, and a number of voids can be easily observed in concrete at meso-scale from X-ray CT images (see [33]). Therefore, spherical/ellipsoidal aggregates are considered for gravel aggregates, while polyhedral aggregates are considered for crushed aggregates. The size distribution of aggregates described by the Fuller curve is summarised in Table 1, and is used in this study [34]. It should be pointed out that only coarse aggregates larger than 2.36 mm are explicitly modelled as meso-scale features and voids with size ranging from 2 mm to 4 mm as presented in [35] are included in the meso-structure of concrete.

<table>
<thead>
<tr>
<th>Sieve size (mm)</th>
<th>Total percentage retained (%)</th>
<th>Total percentage passing (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>12.70</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>9.50</td>
<td>39</td>
<td>61</td>
</tr>
<tr>
<td>4.75</td>
<td>90</td>
<td>10</td>
</tr>
<tr>
<td>2.36</td>
<td>98.6</td>
<td>1.4</td>
</tr>
</tbody>
</table>

The generation process is based on the Monte Carlo sampling method wherein the aggregates and voids are generated from prescribed distributions of their size, shape and volume fraction. A three-level hierarchical method is proposed to reduce the computational cost, and a computationally efficient and versatile in-house program heterogeneous material generator (HMG) has been developed using MATLAB [36]. The detailed algorithms and procedure in generating both 2D and 3D numerical heterogeneous materials can be found in our previous work [1, 32].

Concrete cubic samples cast with a mould in the laboratory with dimensions of 25 mm × 25 mm × 25 mm are generated. Fig. 1 shows the numerically generated models with gravel and crushed aggregates (aggregates in green, voids in red and ITZs in grey). Aggregate gradation in Table 1, aggregate volume fraction $P_{agg}=30\%$, void content $P_{void}=1\%$, aspect ratios for ellipsoidal aggregates and voids (the ratio of the major axis to the minor axis) $R_1=R_2=[1, 2]$, the minimum and maximum edges of the polyhedrons $N_{min}=8$, $N_{max}=16$, minimum space between the edge of an aggregate and the boundary of the concrete specimen $\gamma_1=0.5$ mm and minimum gap width between any two aggregates $\gamma_2=0.5$ mm, are adopted here [35].
2.2 Finite element mesh

The generated meso-structures of concrete illustrated in Fig. 1, are meshed with the pre-processing functionality in commercial FE package ANSYS [37]. A purpose written in-house program was developed to identifying the solid elements of ITZs between mortar and aggregates. The detailed meshing procedure is described as follows:

Firstly, the volume representing aggregates and ITZs $V_{a-I}$ and aggregates only $V_{agg}$, are created. The “overlapping” Boolean operation in the ANSYS pre-processor is applied to separate ITZs domain from aggregates and ITZs domain. Thus, the remaining volume is ITZs, denoted as $V_{ITZ}$. Secondly, the volume representing voids $V_{void}$ and the entire concrete volume $V_{all}$ are created subsequently and the “overlapping” Boolean operation is utilized again to volume domains $V_{ITZ}$, $V_{agg}$, $V_{void}$ and $V_{all}$, which result in separating $V_{mor}$ from $V_{all}$. Finally, the volume representing voids $V_{void}$ is deleted since voids do not contribute to macroscopic mechanical properties of concrete.

The numerical models are meshed with solid hexahedral elements so that more realistic crack paths can be obtained. The ANSYS Parametric Design Language (APDL) programs in combination with ANSYS batch processing are developed to provide a powerful tool of automatic mesh generation. Finite element mesh (element size=0.5mm) corresponding to the concrete with gravel/crushed aggregates and ITZs (aggregates in grey, mortar in blue and ITZs in purple) shown in Fig. 1 is generated and shown in Fig. 2.
3. Constitutive relations

The coarse aggregates usually have a significantly higher strength than mortar, therefore, a linear elastic material model is used to model the aggregates. For mortar and ITZs, concrete damage plasticity model in ABAQUS [38] is employed in the present study. The concrete damage plasticity model assumes that the concrete failure mechanisms are tensile cracking and compressive crushing which is characterised by damage plasticity (see Fig. 3). The cracking is controlled by two hardening variables, $\varepsilon_{\text{pl}}$ and $\varepsilon_{\text{c,pl}}$, linked to failure mechanisms under tension and compression loading, respectively.

In this paper, the analytical expression for normal concrete proposed by Guo and Zhang [39], and later adopted in Chinese Code GB50010 [40] is used for hardening and softening. For both mortar and ITZs under uniaxial tension, the stress-strain response follows a linear elastic relationship until the value of the failure stress $\sigma_{f0}$ which corresponds to the onset of micro-cracking in the concrete, is reached. Beyond the peak stress, the following equation is employed to describe the post-peak softening curve [40].

$$\frac{\sigma}{f} = \frac{\varepsilon}{\varepsilon_{f0}} \left( \frac{\varepsilon}{\varepsilon_{f0}} - 1 \right)^{1/2} + \frac{\varepsilon}{\varepsilon_{f0}}$$  \hspace{1cm} (1)
where \( f_t \) and \( \varepsilon_{t0} \) are the peak stress and peak strain, respectively, and \( \alpha_t \) is a coefficient calculated by \( \alpha_t = 0.312f_t^2 \).

For uniaxial compression, the stress-strain response is linear until the value of initial yield stress \( \sigma_{cy} \) is reached, and the plastic response is characterized by stress hardening followed by strain softening beyond the ultimate stress \( \sigma_{cu} \). The whole relationship is approximated by the following equations [40].

\[
\frac{\sigma_c}{f_c} = \begin{cases} \frac{E_0\varepsilon_c}{f_c}, & \frac{\sigma_c}{f_c} \leq 0.4 \\ \alpha_a \frac{\varepsilon_c}{\varepsilon_{cu}} + (3 - 2\alpha_a)\left(\frac{\varepsilon_c}{\varepsilon_{cu}}\right)^2 + (\alpha_a - 2)\left(\frac{\varepsilon_c}{\varepsilon_{cu}}\right)^3, & \frac{\sigma_c}{f_c} > 0.4 \text{ and } \frac{\varepsilon_c}{\varepsilon_{cu}} \leq 1 \\ \alpha_d \left(\frac{\varepsilon_c}{\varepsilon_{cu}} - 1\right)^2 + \frac{\varepsilon_c}{\varepsilon_{cu}}, & \frac{\varepsilon_c}{\varepsilon_{cu}} > 1 \end{cases}
\]

(2)

where \( f_c \) and \( \varepsilon_{cu} \) are the peak stress and peak strain, respectively, and \( \alpha_a \) and \( \alpha_d \) are coefficients calculated by \( \alpha_a = 2.4 - 0.0125f_c \) and \( \alpha_d = 0.157 f_c^{0.785} - 0.905 \).

It is assumed that the uniaxial stress-strain curves can be converted into stress versus plastic strain curves using the following equations,

\[
\tilde{\varepsilon}_{tp}^l = \tilde{\varepsilon}_{tc}^l + \varepsilon_{t0}^l - \varepsilon_{t0}^{el} \\
\tilde{\varepsilon}_{cp}^l = \tilde{\varepsilon}_{cc}^l + \varepsilon_{c0}^{el} - \varepsilon_{c0}^{el}
\]

(3)

(4)

where \( \tilde{\varepsilon}_{tp}^l \) and \( \tilde{\varepsilon}_{cp}^l \) are equivalent plastic strain in tension and compression, \( \tilde{\varepsilon}_{tc}^l \) and \( \tilde{\varepsilon}_{cc}^l \) are cracking strain and inelastic strain, and \( \varepsilon_{t0}^l, \varepsilon_{c0}^{el}, \varepsilon_{t}^{el} \) and \( \varepsilon_{c}^{el} \) are calculated using Equations (5) and (6),

\[
\varepsilon_{l}^{el} = \frac{\sigma_{l}}{E^{el}}, \varepsilon_{w}^{el} = \frac{\sigma_{w}}{E^{el}}
\]

(5)

(6)

where \( d_l \) and \( d_c \) are damage variables in tension and compression, which evolves monotonically from 0, representing the undamaged material, to 1 which represents total loss of strength.
The stress-strain relations (σ-ε) under uniaxial tension and compression loading are given by Equations (7) and (8), respectively,

\[
\sigma_i = (1 - d_i) E_o (\varepsilon_i - \tilde{\varepsilon}_i^{pl})
\]

\[
\sigma_c = (1 - d_c) E_o (\varepsilon_c - \tilde{\varepsilon}_c^{pl})
\]

where the strains in tension and compression can be represented as follows,

\[
\varepsilon_i = \tilde{\varepsilon}_i^{ck} + \varepsilon_i^{el}, \varepsilon_c = \tilde{\varepsilon}_c^{in} + \varepsilon_c^{el}
\]

In order to account for different effects under tension and compression loadings, two damage criteria are used: one for tension and a second for compression. Substituting Equations (3) and (4) into Equation (9) and using Equations (7) and (8) results in

\[
d_i = 1 - \frac{\sigma_i / E_o}{\tilde{\varepsilon}_i^{pl} (1/b_i - 1) + \sigma_i / E_o}
\]

\[
d_c = 1 - \frac{\sigma_c / E_o}{\tilde{\varepsilon}_c^{pl} (1/b_c - 1) + \sigma_c / E_o}
\]

where \(b_i\) and \(b_c\) are constant factors extracted from experimental tests, and are calculated as \(b_i = \tilde{\varepsilon}_i^{pl} / \varepsilon_i^{ck}\), \(b_c = \tilde{\varepsilon}_c^{pl} / \varepsilon_c^{in}\). Here the values 0.1 and 0.7 are selected for \(b_i\) and \(b_c\), respectively, as suggested by Britel et al. [41].

(a) Tension

(b) Compression

Fig. 3. Uniaxial stress-strain curve with damage
4. Finite element modelling

3D concrete specimens with spherical aggregates and voids (25mm×25mm×25mm concrete cubic, \( P_{\text{agg}}=30\% \), \( P_{\text{void}}=1\% \), \( \gamma_1=\gamma_2=0.5\text{mm} \)) were first loaded under uniaxial compression and tension (see Fig. 4). The loading was displacement-controlled with zero prescribed vertical (X-direction) displacements at nodes on the bottom surfaces and non-zero vertical displacements at nodes on the top surfaces. Horizontal displacements for the same nodes are left free, except for the nodes at the right lower corner of the specimens, which are fixed to prevent rigid body translation. The material properties used in this study are determined based on the data from relevant publications [9, 12], and are listed in Table 2. In addition, five other parameters are needed for damage-plasticity model used in this study: dilation angle: 35°, flow potential eccentricity: 0.1, biaxial/uniaxial compression plastic strain ratio: 1.16, invariant stress ratio: 0.667, viscosity parameter: 0.0005 are adopted for both mortar and ITZs. Tensile and compressive stress data are provided as a tabular function of strain, which is directly obtained from the constitutive relation of mortar and ITZs. The damage variables defined by Equations (10) and (11) are defined as a tabular function of cracking strain and inelastic strain for tension and compression, respectively.

![Specimen dimensions, loading and boundary conditions](image1)

(a) Uniaxial compression (b) Uniaxial tension

Fig. 4. Specimen dimensions, loading and boundary conditions

The commercial software ABAQUS/Explicit was used for finite element analysis. The explicit method in ABAQUS was originally developed to solve dynamic problems, so it is important that the inertial forces do not affect mechanical responses and provide unrealistic dynamic results when performing quasi-static analysis. In
principle, the loading time should be long enough to minimise any dynamic effects but not too long to cause excessive computational cost. After a trial and error analysis, loading displacement \( d = 0.1 \) mm, loading time \( t = 0.1 \) s were found to be long enough to ensure the quasi-static loading condition [1, 42].

<table>
<thead>
<tr>
<th>Material properties</th>
<th>Aggregate</th>
<th>Mortar</th>
<th>ITZ</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus ( E ) (GPa)</td>
<td>70</td>
<td>25</td>
<td>22</td>
</tr>
<tr>
<td>Poisson’s ratio ( \nu )</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
</tr>
<tr>
<td>Density ( \rho ) (kg/m(^3))</td>
<td>2600</td>
<td>2200</td>
<td>2200</td>
</tr>
<tr>
<td>Tensile strength (MPa)</td>
<td>/</td>
<td>4</td>
<td>3</td>
</tr>
<tr>
<td>Compressive strength (MPa)</td>
<td>/</td>
<td>45</td>
<td>35</td>
</tr>
</tbody>
</table>

5. Simulation results

5.1 Uniaxial compression modelling

5.1.1 Stress strain behaviour

A typical 3D concrete specimen as described in section 4 is modelled loaded under uniaxial compression. The numerical simulation of the concrete specimen loaded under uniaxial compression with 1,092,481 finite elements and 190,627 nodes in this study takes about 6 hours by parallel computation with 64 CPUs. Fig. 5 shows the predicted mean stress-strain curves in X direction for a 3D heterogeneous concrete subjected to uniaxial, monotonic compression loading, typical experimentally observed response [43] and another numerical result [44]. The mean stress is calculated as the sum of reaction force of nodes on the bottom surface divided by the cross-section area of the specimen.

It can be seen that the stress-strain curve predicted in this study is consistent and in good agreement with those from experimental test and the other numerical work. The curves show that typical concrete behaviour is characterised by an initial elastic region, a nonlinear hardening range before the peak stress, and a following softening branch. However, given the wide variation in the experimental data, and the specimens are of different aggregate and void spatial distribution, etc, calibration of
the model to represent the results of a single experimental test or other numerical work is not productive. It should also be noted that the stress-strain curve predicted shows more brittle behaviour than the experimental result, this could be due to the delayed initiation of micro-cracks or increasing creep effects at high stress levels measured in tests. It is still unclear as there are no experiments in which micro-crack initiation and evolution in the pre-peak phase has been properly investigated.

![Stress-strain curves under uniaxial compression](image)

**Fig. 5. Stress-strain curves under uniaxial compression**

Mean stress-strain curves in axial (X axis) and lateral directions (Y and Z axes), and the volumetric stress-strain curve are shown together in Fig. 6. The lateral strains ($\varepsilon_y$ and $\varepsilon_z$), are calculated by finding the mean value of all the nodal displacements on the two opposite surfaces perpendicular to corresponding axes and dividing their relative displacements by the specimen size. The volumetric strain is approximated as the sum of axial strain ($\varepsilon_x$) and lateral strains ($\varepsilon_y$ and $\varepsilon_z$): $\varepsilon = \varepsilon_x + \varepsilon_y + \varepsilon_z$. It could be observed that the lateral strains (right part in Fig. 6) evolve approximately as the Poisson relation times the axial strain before reaching the peak stress, then increase fast and exceed the prescribed strain in the loading direction in the softening range. The volumetric strain decreases first due to the contraction under compression, and then increases after crack initiation and propagation at the later loading stage. These results agree qualitatively with typical experimental data obtained by Van Mier [45], and support the realism of the proposed modelling approach.
5.1.2 Cracking evolution

In order to illustrate the cracking process under compression, three special loading points, corresponding to one in the hardening range, one at peak stress and another at late softening range are investigated, the results are shown in left, middle and right columns in Fig. 7, respectively. The compressive and tensile damage in the front and rear views of the specimen clearly shows the cracking and localization process during the loading. The different views of cracking patterns seen from the front and rear views are attributed to the heterogeneous random distribution of aggregates and voids. The reason for the emergence of tensile damage (see Fig. 7(c) and Fig. 7(d)) in compression is the material heterogeneity with aggregates and voids located randomly. The vertical loading on the top and bottom of aggregates results in generating inclined compressive stress which leads to the emergence of horizontal tensile stress between aggregates. It is worth noting that the diagonal compression failure predicted is associated with the compressive law where more brittle behaviour is assumed, while experimental tests sometimes show multiple vertical cracks before the development of a single failure plane.

Due to the relative weakness of aggregate-mortar interfaces, compressive damage starts at hardening stage (see left column in Fig. 7(a-b)) and tensile damage starts at peak stress in aggregate-mortar interfaces (see middle column in Fig. 7(c-d)). Around the peak stress, damage increases and micro-cracks (mostly the cracks in aggregate-mortar interfaces) start coalescing (see middle column in Fig. 7). With the loading progressing into the softening region, both the compressive and tensile damage
accelerate and the cracks propagate through mortar in the late softening stage (see right column in Fig. 7). The predicted cracking evolution process is found to be in agreement with both experimental and numerical work in elucidating mechanisms of the micro-cracking and damage evolution in compression [44, 45].

Fig. 7. Cracking evolution at various loading stages under uniaxial compression
Hardening (left column), peak stress (middle column), softening (right column)
5.2 Uniaxial tension modelling

5.2.1 Stress strain behaviour

In this section, the same finite element model used in uniaxial compression is numerically tested under uniaxial tension, and all the other parameters are fixed to the values used in section 5.1. A typical simulation of concrete specimen under uniaxial tension loading with the same number of elements and nodes takes about 5 hours by parallel computation with 64 CPUs. Fig. 8 shows a good correlation of stress-strain curve of a 3D heterogeneous concrete subjected to uniaxial, monotonic tension loading predicted in this study, with experimentally observed response [46] and the result from another numerical work [32]. The mean stress is obtained by summing the nodal reaction forces in the constraints and dividing by the cross-section area of the specimen. They are qualitatively similar to each other with a clear peak and sharp initial post-peak drop followed by a long shallow tail. However, one should not compare the curves quantitatively as they describe specimens of different distribution, volume fraction of aggregates and voids, etc.

![Image](image_url)

**Fig. 8.** Stress-strain curves under uniaxial tension

5.2.2 Cracking evolution

The detailed cracking patterns under uniaxial tension at peak stress, initial softening and late softening are presented in left, middle and right columns in Fig. 9, respectively. The tensile and compressive damage in both front and rear views of the specimen are used to clearly demonstrate the cracking initiation and propagation during the loading.
Fig. 9. Cracking evolution at various loading stages under uniaxial tension
Peak stress (left column), initial softening (middle column), late softening (right column)
It can be seen that micro-cracks start emerging after reaching the peak stress (see left column in Fig. 9), and tensile damage starts developing especially at the aggregate-mortar interfaces perpendicular to the loading direction (see middle column in Fig. 9). As the loading displacement increases, some micro-cracks coalesce into dominant cracks, while the other cracks arrest due to stress redistribution (see right column in Fig. 9). It should also be noted that a much smaller number of elements are under compressive damage in tension loading (Fig. 9(c) and Fig. 9(d)) compared to the elements under tensile damage for compression case (see Fig. 7(c) and Fig. 7(d). It indicates that the compression results are associated with both tensile and compressive behaviour of the meso-phases in concrete, while the tension test of meso-structural concrete is dominated by the tensile behaviour of each meso-phase.

5.3 Effect of material heterogeneity

The effect of material heterogeneity is investigated by performing both compression and tension simulation on three concrete specimens with different aggregate and void spatial distribution while all the other parameters are fixed to the values used in sections 5.1 and 5.2. As shown in Fig. 10(a) for tension and Fig. 10(b) for compression, the stress-strain curves share an almost identical response of monotonic increase in the pre-peak range, however, the difference in peak strength is about 4% for tension and 6% for compression, and obvious differences are also observed between the post-peak responses.

Fig. 11 and Fig. 12 compare the failure cracking patterns for the three different samples under compression and tension, respectively. Compressive damage and tensile damage are used to illustrate the cracking patterns in Fig. 11 and Fig. 12, respectively. The different figures shown in Fig. 11 and Fig. 12 demonstrate that the distribution of aggregates and voids has a significant effect on the failure cracking patterns for both uniaxial compression and tension. Two typical macro-crack patterns for uniaxial tension as presented by image-based modelling [47] and cohesive zone modelling [32] are also observed in this study: Type I cracking with only one dominant crack (see Fig. 12(a) and Fig. 12(b)) and Type II cracking with two or more dominant cracks (see Fig. 12(c)). A larger load-carrying capacity in softening range is observed for type II cracking (sample 3 in Fig. 10(b)). It could be explained by the emergence of multiple concurrently growing macro-cracks which leads to increased toughness.
Apparently, crack propagation and stress-strain response in concrete under both tension and compression are affected by its highly disordered meso-structure. The results obtained in this study indicate that conclusions based on a small number of analyses may be drawn for the pre-peak range; however, it should be taken carefully to draw conclusions for the peak strength and post-peak response on the basis of a small number of analyses. Therefore, it is necessary to do a statistical analysis if the peak strength and softening process are what we are concerned. Further study will
concentrate on developing parallel computing algorithms to reduce computational cost and improve efficiency for statistical analysis of damage and failure of a large number of 3D concrete specimens.

5.4 Effect of void content

The effect of void content on the fracture behaviour is investigated by fixing the positions of aggregates and aggregate volume fraction, but varying the void content. All the other geometric and material parameters except the void content are fixed to the values used in Sections 5.1 and 5.2. As shown in Fig. 13, the effect of void content for both uniaxial tension and compression on the resulting stress-strain curves is pronounced, especially for peak and post-peak range. The load-carrying capacity decreases as the void content increases for both compression and tension. We suggest that this is because the voids enable the cracks to propagate easily through them so that the samples fail quickly. It clearly shows that the voids which exist in the concrete should not be neglected when analyzing the mechanical properties and fracture of concrete. It should also be noted that the distribution of voids may also have some effect on the resulting stress-strain curves, and a quantitative prediction could only be obtained by statistical analysis.

![Stress-strain curves for concrete specimens with different void content](image)

(a) Uniaxial compression
(b) Uniaxial tension

Fig. 13. Stress-strain curves for concrete specimens with different void content

The void distribution for three specimens with same aggregate distribution and aggregate volume fraction ($P_{agg}=30\%$), but different void content, i.e. 0%, 1% and 2% is shown in Fig. 14. Fig. 15 and Fig. 16 also show that the effect of void content on the cracking patterns is pronounced. This is not unrealistic as one might expect voids to provide an easy path for cracks to propagate. It is also clearly illustrated in Fig. 15 and Fig. 16 that more voids become connected with the cracking surface with the
increase of void content. For both tension and compression, it seems that cracks tend to propagate along voids and neighbourhood of aggregates, preferable paths are chosen if this aggregate is relatively large. So, we suggest that it is important to consider voids which have rarely been considered in meso-structural of concrete when analyzing the failure and damage behaviour.

Fig. 14. Void distribution in concrete specimens with different void content

Fig. 15. Cracking patterns for concrete specimens with different void content under compression ($P_{agg}=30\%$)

Fig. 16. Cracking patterns for concrete specimens with different void content under tension ($P_{agg}=30\%$)
6. Conclusions

A computational method for damage and failure analysis of numerically generated synthetic 3D heterogeneous concrete is developed. It is validated qualitatively with available publications of stress-strain curves and 3D damage and cracking evolution under both tension and compression. In general, the model represents well the fundamental characteristics of concrete tensile and compressive responses, which allows us to tackle with confidence more complex concrete structures. The model is capable of capturing localization phenomena, from micro-cracking through crack coalescence to ultimate failure, including bridging and branching mechanisms. The aggregate and void distributions are demonstrated to have a pronounced effect on both the macroscopic stress-strain behaviour and the cracking patterns for compression and tension. The load-carrying capacity decreases as the void content increases in both compression and tension. It is further shown that the void content has a large effect on the failure patterns. This leads to the conclusion that voids should be considered in meso-scale fracture modelling of concrete. Further study will concentrate on the behaviour of concrete under complex loading conditions, i.e. triaxial stress fields, present in different locations of engineering components, as means for deriving improved constitutive laws for continuum-based modelling of concrete structures. An important element of this future research is statistical analysis of the effects of shape, size, gradation, spatial distribution, volume fraction of aggregate and void on the concrete behaviour, for which parallel computing algorithms are required.

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References


A Non-matching Finite Element-Scaled Boundary Finite Element Coupled Method for Linear Elastic Crack Propagation Modelling

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8.1 Statement of own contributions in joint authorship

- Main research technology development;
- Preparation of tables and figures, and writing of the manuscript;
- In-house MATLAB programs development for coupling FEM and SBFEM;
- Numerical modelling by developed in-house programs;
- Data processing and analysis;
- Interpretation of results.

8.2 Paper in the research context

This paper proposes a new computational technology named non-matching FE-SBFE coupled method to simulate crack propagation problems based on the linear elastic fracture mechanics. The idea initiates from the FEM non-matching method used in fracture problems. In order to reduce the computational cost, materials can be naturally divided into two parts, the local crack-tip part modelled with fine meshes, and the rest global part without cracks modelled with coarse meshes. In the proposed
method, a similar concept as zero-thickness CIEs used in Chapter 2 and 3 but specified without nonlinear response is adopted. Taking the advantage that the SBFEM offers a very high accuracy in calculating stress intensity factors with much fewer degrees of freedom, the SBFE subdomain boundary is coupled with the surrounding FE mesh boundary through the virtual zero-thickness interfaces. The accuracy and effectiveness of the developed computational technology are demonstrated by modelling a variety of fracture problems.

This Chapter is an exact copy of the journal paper referred to above.
(See Paper VI as follows)
A non-matching finite element-scaled boundary finite element coupled method for linear elastic crack propagation modelling

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A B S T R A C T
A novel method coupling the scaled boundary finite element method (SBFEM) and the finite element method (FEM) is developed for linear elastic fracture modelling. A very simple but effective remeshing procedure based on the FE mesh only is used to accommodate crack propagation. The crack-tip region is modelled by an SBFE subdomain whose semi-analytical displacement solutions are used to extract accurate stress intensity factors. The SBFE subdomain is coupled with the surrounding FE mesh through virtual interfaces so that non-matching nodal discretisations of the shared boundaries can be used and only one SBFE subdomain is needed at a crack-tip. A few plane problems are modelled to validate the new method.

1. Introduction

There exist inherently various defects and flaws in engineering materials and structures from nano-, micro- to meso-scales. Under certain external loadings, these small-scale defects and flaws can develop into macro-scale cracks, whose initiation and propagation may severely affect the structural integrity and safety. Therefore, understanding crack propagation behaviour by laboratory experiments and numerical simulations has attracted tremendous attention in last five decades. This paper is focused on numerical modelling of crack propagation problems.

The difficulties and challenges of numerical modelling of crack propagation are reflected by numerous numerical methods developed so far, e.g., the finite element method (FEM), the boundary element method (BEM), the meshless or meshfree method, and more recently, the extended FEM (XFEM). The FEM is the most popular numerical method in simulating crack propagation because of the high generality and flexibility of the method in modelling structures with complex geometries, various boundaries and loading conditions [1–3]. However, when the FEM is used to simulate crack propagation, very fine crack-tip meshes or special elements are needed to calculate accurate stress intensity factors (SIFs) for crack propagation. This makes remeshing difficult. The BEM is another popular method that has been widely used to model fracture problems [4–7]. The modelled spatial dimensions are reduced by one because only boundaries are discretised, which makes remeshing much simpler. However, the BEM is applicable only to problems where Green’s functions can be derived, which restricts its wide applicability [8]. The meshless or meshfree method [9] models a domain with boundaries and scattered nodes only. Nodal moving rather than remeshing around the crack-tip is carried out as the crack propagates. This method can calculate accurate SIFs but the computational cost is generally higher than the FEM [10]. In the XFEM, the displacement discontinuity across the crack faces is taken into account by adding discontinuous functions to the shape functions to avoid remeshing [11–14]. Extra terms of enrichment functions are needed to capture different crack-tip singularities. This makes the formulation of shape functions complicated and the numerical integration becomes involving and less accurate [14,15]. Many special crack-tip elements with built-in singularities, e.g. quarter point elements [16], hybrid Trefftz elements [17], hybrid crack elements (HCE) [18–20] have also been developed in the FEM, BEM and XFEM.

A more recent alternative is the scaled boundary finite element method (SBFEM). It is a semi-analytical method developed by Song and Wolf [21,22] in the late 1990s. This method not only combines the advantages of FEM and BEM but also exhibits additional advantages, e.g., it discretises boundaries only and the spatial dimension
is reduced by one like the BEM, but requires no fundamental solutions; it avoids singular integrals and extends the BEM’s applicability considerably [23–25]. It is very efficient in modelling problems with discontinuities and singularities because of its semi-analytical nature. Ooi and Yang [26,27] recently developed a hybrid FE–SBFE method capable of automatically modelling multiple crack propagation. The hybrid method retains the advantages of SBFEM such as its high accuracy in calculating SIFs and that of FEM such as its flexibility in modelling complicated geometries. However, several crack-tip SBFE subdomains are needed in the hybrid method to maintain the matching nodal discretisation with surrounding finite elements. New methods coupling BEM and SBFEM [28,29] and XFEM [30] have also been developed in computational fracture mechanics.

In the domain decomposition technique, a domain is divided by virtual interfaces into independent parts which can be meshed separately, and non-matching nodal discretisations can be used on the two sides of the virtual interfaces [31–34]. The displacement compatibility across the virtual interfaces can be ensured by using sufficiently high stiffness on the interfaces [35–37]. In fracture problems, a domain can be conveniently divided into two parts, the local crack-tip part modelled with fine meshes to calculate accurate SIFs, and the rest global part without cracks modelled with coarse meshes. Using the non-matching technique, only the local crack-tip part needs to be remeshed/refined as the crack propagates (e.g., [37–39]), whereas the global part often needs to be remeshed as well when the matching meshes are used [3,40].

This study proposes a non-matching SBFEM–FEM coupled method to simulate quasi-static crack propagation problems based on the linear elastic fracture mechanics (LEFM). In this method, a very simple remeshing procedure based on FE meshes only is used with accurate SIFs calculated by crack-tip SBFE subdomains. The main difference between the present method and the previous hybrid FE–SBFE method [26] is that in the present method, the SBFE subdomain boundary is coupled with the surrounding FE mesh boundary through virtual interfaces so that the nodal discretisations of the two boundaries can be different and only one SBFE subdomain is needed for one crack, whereas in the previous method, several subdomains are needed to maintain the matching nodal discretisation. Compared with the non-matching method based on FEM only, this method offers higher accuracy in calculating SIFs with much fewer degrees of freedom (DOF) due to the semi-analytical nature of SBFEM.

2. The non-matching SBFEM–FEM coupled method

2.1. The scaled boundary finite element method

In the SBFEM, a domain is divided into subdomains whose shapes and areas can be very different from one to another. Fig. 1 illustrates a two-dimensional (2D) subdomain, which is represented by scaling a defining curve $\mathcal{S}$ relative to a scaling centre. A normalised radial coordinate $\xi$ is introduced, varying from zero at the scaling centre to unit on $\mathcal{S}$. A circumferential coordinate $\theta$ is defined around the defining curve $\mathcal{S}$. Thus, $\xi$ and $\theta$ form a local
coordinate system used in the subdomain and are related to the Cartesian coordinates \((x, y)\) by the transformation relations [21]
\[
x = x_0 + \xi x_1(s) \quad y = y_0 + \xi y_1(s)
\]
(1)

Only the subdomain boundary is discretised by nodes. As in isoparametric finite element method, the displacement vector at any point \((\zeta, s)\) in a subdomain can be approximated by
\[
\mathbf{u}(\zeta, s) = \mathbf{N}_b(\zeta, s)\mathbf{u}_b
\]
(2)
where \(\mathbf{u}_b\) is the nodal displacement vector of the subdomain, and the shape function matrix \(\mathbf{N}_b\) is given by [26,41]
\[
\mathbf{N}_b(\zeta, s) = \mathbf{N}_b(s)\Phi(\zeta)^{-1}
\]
(3)
where \(\mathbf{N}_b(s)\) is the one-dimensional shape function matrix as in FEM, \(\Phi(s) = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)\) and \(\Phi = \{\phi_1, \phi_2, \ldots, \phi_n\}\) are the subset of positive eigenvalues and modal displacements obtained from solving an eigenvalue problem [41], and \(n\) is the DOFs of the subdomain.

The stress field \(\sigma(\zeta, s)\) in a subdomain is given by
\[
\sigma(\zeta, s) = \mathbf{D}^1(\zeta, s)\left[\sum_{i=1}^{n} c_i z_i^{2(\zeta-1)}\phi_i\right] + \mathbf{D}^2(\zeta, s)\left[\sum_{i=1}^{n} c_i z_i^{2(\zeta_i-1)}\phi_i\right]
\]
(4)
where \(c_i\) are constants dependent on boundary conditions, \(\mathbf{D}\) is the elastic matrix, and \(\mathbf{B}^1(s)\) and \(\mathbf{B}^2(s)\) are strain–displacement matrices [41].

The stiffness matrix of the subdomain with respect to the boundary DOFs is [26]
\[
\mathbf{K}_b = \mathbf{E}^0\mathbf{\Phi}(\zeta)\mathbf{\Phi}^{-1} + \mathbf{E}^1^T
\]
(5)

where \(\mathbf{E}^0\) and \(\mathbf{E}^1\) are matrices dependent on the geometry and material properties of the subdomain only.

It is clear from Eqs. (2)–(4) that both the displacement and the stress solutions in a subdomain are analytical in the radial direction \((\zeta)\), and approximate in the circumferential direction \((s)\) in the FEM sense.

2.2. Coupling SBFEM and FEM with non-matching meshes

Fig. 2a shows a domain \(\Omega\) with a crack, modelled by a FE part \(\Omega_{FE}\) away from the crack tip and an SBFE subdomain \(\Omega_{SB}\) surrounding the crack tip. Different mesh densities in \(\Omega_{FE}\) and \(\Omega_{SB}\) result in non-matching nodal discretisations along the shared boundary. Fig. 2b shows the virtual interface of zero in-plane thickness (the dashed line), which coincides with the defining curve \(S\) (with \(z = 1\)) of the SBFE subdomain \(\Omega_{SB}\). The gap between the defining curve \(s\), the virtual interface \(S\), and the surrounding FE mesh are shown in Fig. 2b only for illustration purpose.

For any point with the circumferential coordinate \(s\) on the virtual interface \(S\), there is a point 1 on the FE boundary and a point 2 on the SBFE boundary, possessing the same coordinates (plotted as white triangles in Fig. 2b). The displacement vector \(\mathbf{d}_i(s)\) of point 1 in the global coordinate system can be calculated by
\[
\mathbf{d}_i(s) = \mathbf{N}_i(s)\mathbf{u}_i
\]
(6)
where \(\mathbf{u}_i\) is the nodal displacement vector of the finite element \(i\) in which the point 1 is located, and \(\mathbf{N}_i(s)\) is the shape function matrix at point 1 in the finite element \(i\), whose components are functions of
The two local parametric coordinates of point 1 in the finite element

\[ f \]

The displacement vector \( \mathbf{d}_2(s) \) of point 2 can be obtained by Eq. (2) as

\[ \mathbf{d}_2(s) = \mathbf{N}_b(s) \mathbf{u}_b \]

where \( \mathbf{N}_b(s) \) are functions of the circumferential coordinate \( s \) only as \( \zeta = 1 \) on the defining curve \( S \) (see Eq. (3)).

To simplify the derivation, Eqs. (6) and (7) can be rewritten by expanding \( \mathbf{u}_f, \mathbf{u}_b, \mathbf{N}_f(s) \) and \( \mathbf{N}_b(s) \) into the global DOFs as

\[ \mathbf{d}_1(s) = \mathbf{N}_f(s) \mathbf{u} \]

\[ \mathbf{d}_2(s) = \mathbf{N}_b(s) \mathbf{u} \]

where \( \mathbf{u} \) is the nodal displacement vector of the whole model with \( N \) DOFs, and \( \mathbf{N}_f(s) \) and \( \mathbf{N}_b(s) \) are now both \( 2 \times N \) matrices.

**Fig. 7.** Vertical displacement contours from structured \( 20 \times 40 \) mesh (\( \times 10^{-11} \)).

**Table 1**

Errors of \( K_I \) for the edge-cracked plate under mode-I loading.

<table>
<thead>
<tr>
<th>FEM</th>
<th>No. elements</th>
<th>No. DOF</th>
<th>Error (( K_I ), %)</th>
<th>X-FEM</th>
<th>No. elements</th>
<th>No. DOF</th>
<th>Error (( K_I ), %)</th>
<th>Present method</th>
<th>No. elements</th>
<th>No. DOF</th>
<th>Error (( K_I ), %)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 x 8</td>
<td>94</td>
<td>25.0</td>
<td>5 x 7</td>
<td>136</td>
<td>18.5</td>
<td>8 x 8</td>
<td>222</td>
<td>7.2</td>
<td>8 x 16</td>
<td>442</td>
<td>3.6</td>
</tr>
<tr>
<td>8 x 16</td>
<td>314</td>
<td>14.3</td>
<td>9 x 15</td>
<td>368</td>
<td>8.4</td>
<td>16 x 32</td>
<td>1266</td>
<td>1.7</td>
<td>31 x 31</td>
<td>20 x 40</td>
<td>1870</td>
</tr>
<tr>
<td>16 x 32</td>
<td>1138</td>
<td>7.6</td>
<td>17 x 31</td>
<td>1216</td>
<td>3.7</td>
<td>16 x 32</td>
<td>1266</td>
<td>1.7</td>
<td>20 x 40</td>
<td>1870</td>
<td>1.3</td>
</tr>
<tr>
<td>20 x 40</td>
<td>1742</td>
<td>4.2</td>
<td>21 x 39</td>
<td>1832</td>
<td>2.9</td>
<td>20 x 40</td>
<td>1870</td>
<td>1.3</td>
<td>40 x 40</td>
<td>4450</td>
<td>0.8</td>
</tr>
<tr>
<td>32 x 64</td>
<td>4322</td>
<td>4.0</td>
<td>33 x 63</td>
<td>4448</td>
<td>1.7</td>
<td>44 x 40</td>
<td>4450</td>
<td>0.8</td>
<td>40 x 40</td>
<td>4450</td>
<td>0.8</td>
</tr>
</tbody>
</table>

**Fig. 8.** Effects of the SBFE subdomain shape.

The relative displacements of points 1 and 2, with one component along the virtual interface and another normal to it, are
\[ \mathbf{d}(s) = L(s)\left(\mathbf{d}_1(s) - \mathbf{d}_2(s)\right) \] (10)
where
\[ L(s) = \begin{bmatrix} \cos \theta(s) & -\sin \theta(s) \\ \sin \theta(s) & \cos \theta(s) \end{bmatrix} \] (11)
is the coordinate transformation matrix and \( \theta(s) \) is the inclination angle of the virtual interface at the considered point and measured clockwise from the \( s \) direction to the positive \( x \)-axis (see Fig. 2b).

Assuming that the relative displacements are sustained by two virtual springs with stiffness coefficients \( k_s \) along the virtual interface and \( k_n \) normal to it, the force vector on a unit length transferred by the springs is
\[ \mathbf{P}(s) = D_c \mathbf{d}(s) \] (12)
with
\[ D_c = \begin{bmatrix} k_s \\ k_n \end{bmatrix} \] (13)

The introduction of the virtual interface and the virtual springs leads to artificial gaps or penetrations along the shared boundary, and spurious potential energy which should be minimised. The potential energy on the whole virtual interface is
\[ II = \int_s P(s)\mathbf{d}(s)ds \] (14)
Substituting Eqs. (10)–(12) into Eq. (14) and using Eqs. (8) and (9) result in...
The system stiffness matrix is then obtained by assembling Eqs. (5), (18) and the stiffness matrices of all the finite elements. The spring stiffness coefficients \( k_s \) and \( k_n \) play a vital role in the accuracy of this coupling procedure. Too high values may lead to ill-posedness of the system equations and too low values cannot ensure displacement continuity across the virtual interface. The following equation is proposed in [35] as a guide

\[
k_s = k_n = k = \frac{c(1 - \nu)}{b(1 + \nu)(1 - 2\nu)} E
\]

where \( E \) and \( \nu \) are the Young’s modulus and Poisson’s ratio, \( b \) is the characteristic size of elements, and \( c \) is taken as 10–100 from the experience in [35].

### 3. Fem-based remeshing procedure

When a crack is judged to propagate, a very simple, local remeshing procedure similar to the one in [43,44] is used to accommodate its propagation. Fig. 3a shows a crack-tip mesh at the previous loading step. The new crack-tip location is first found from the crack propagation direction, which is calculated by the maximum circumferential stress criterion in this study [45]. The closest node to the new crack-tip is then dragged to its position and becomes the new crack-tip node, and the old crack-tip node is split into two nodes to form the new crack (Fig. 3b). All the 4-noded elements connected with the new crack-tip node are then triangularised (Fig. 3c). If the internal angle of any crack-tip triangular elements is over 85° (e.g., \( \theta_1 \) and \( \theta_2 \) in Fig. 3c), its nodal connectivity is changed for a better-shaped crack-tip mesh (Fig. 3d) which will be used as the initial mesh for remeshing in the next loading step.
4. Calculation of stress intensity factors

The shaded area covered by the crack-tip elements in Fig. 3d is replaced by a SBFE subdomain to accurately calculate the SIFs, and it is illustrated in Fig. 4.

In Fig. 4, the scaling centre of the cracked subdomain is conveniently placed at the crack-tip. The SIFs can be extracted directly from either the asymptotic displacement solutions [46] or the stress solutions [23]. In this study, the displacement solutions are used. The relations between the SIFs and the crack-tip displacement field with a local coordinate system shown in Fig. 4 are given as follows [47]

\[
\begin{align*}
    u_x(r, \theta) &\approx \frac{K_i}{G} \sqrt{\frac{r}{2\pi \rho}} \cos \frac{\theta}{2} \left[ \frac{1}{2} (\kappa - 1) + \sin^2 \frac{\theta}{2} \right] \\
    u_y(r, \theta) &\approx \frac{K_{ii}}{G} \sqrt{\frac{r}{2\pi \rho}} \sin \frac{\theta}{2} \left[ \frac{1}{2} (\kappa + 1) + \cos^2 \frac{\theta}{2} \right] \\
\end{align*}
\]

where \( G \) is the shear modulus and \( \kappa \) is given by

\[
\kappa = \begin{cases} 
3 - 4v & \text{for plane strain} \\
(3 - v)/(1 + v) & \text{for plane stress} 
\end{cases}
\]

in which \( v \) is the Poisson’s ratio.

Using \( \theta = \pi \) to decouple \( K_i \) and \( K_{ii} \) in Eqs. (20) and (21), and \( r = r_0 \) where \( r_0 \) is the length from the crack-tip to the crack-mouth node at \( \theta = \pi \), the SIFs are obtained as

\[
\begin{align*}
    \left\{ \begin{array}{l}
    K_i \\
    K_{ii}
    \end{array} \right\} &= \frac{2G}{\kappa + 1} \left( \frac{2\pi}{r_0} \left[ u_x(r_0, \pi) \right] \right) \\
\end{align*}
\]
where \( u_l(r_0, \pi) \) and \( u_l(r_0, \pi) \) can be extracted from the displacement field.

\[
\mathbf{u}(z, s) = \mathbf{N}_b(s) \sum_{i=I}^{II} c_i \mathbf{v}_i
\]

(24)

in which \( I \) and \( II \) are the two modes with \( \lambda_i = 0.5 \) that correspond to mode-I and mode-II deformations [46].

5. Numerical examples

Six two-dimensional problems corresponding to mode-I, mode-II and mixed-mode fracture are modelled to validate the developed method and demonstrate its capability. The quasi-static loading condition is assumed for all the examples.

5.1. An edge-cracked plate under mode-I loading

The first example is an edge-cracked plate subjected to a remote unit stress (\( \sigma = 1 \)) applied on the top and bottom. The geometry, boundary and loading conditions are shown in Fig. 5a.

The exact solution of the mode-I SIF is given by [48]

\[
K_I = C\sigma \alpha \pi
\]

(25)

where \( C \) is a finite geometry correction factor

\[
C = 1.12 - 0.231 \left( \frac{a}{W} \right) + 10.55 \left( \frac{a}{W} \right)^2 - 21.72 \left( \frac{a}{W} \right)^3 + 30.39 \left( \frac{a}{W} \right)^4
\]

(26)

in which \( a \) is 3.5 and \( W \) is 7.0 in this example, and thus the exact solution is \( K_{Ie} = 9.37. \)

To investigate the effects of the coupling parameter \( k \) in Eq. (19), structured FE meshes are used first. Fig. 5b shows a mesh with \( 20 \times 40 \) 4-noded quadrilateral elements. The FE-SBFE coupled mesh is shown in Fig. 5c, with the detailed region at the crack-tip highlighted in Fig. 5d.

Fig. 6 plots the errors of \( K_I \) from three meshes as the virtual spring stiffness coefficient \( k \) varies. It is reconfirmed that too high or too low values of \( k \) lead to unsatisfactory accuracy. For this example, it is found that \( k = 10^3E - 10^{10}E \) results in around 1\% error in \( K_I \). From the vertical displacement contours shown in Fig. 7 (\( 20 \times 40 \) mesh), the use of virtual interface between the FE and SBFE meshes does not affect the displacement continuity. For this reason, \( k = 100E \) is used in all the following examples, corresponding to \( c = 26 \) in Eq. (19).

Fig. 8 shows the shape effects of the SBFE subdomain on the accuracy of \( K_I \) using the \( 20 \times 40 \) mesh as an example. All the SBFE subdomains lead to less than 3\% error, indicating that \( K_I \) is almost independent of the shape of the SBFE subdomain. This is important because the remeshing procedure may lead to irregular SBFE shapes similar to those in Fig. 8.

Table 1 compares the relative errors of \( K_I \) for five structured meshes using the FEM, the XFEM and the method proposed in this paper. The \( J \)-integral approach in Abaqus [49] and a domain interaction integral method [50] are used to calculate \( K_I \) by the FEM and the XFEM respectively. The results are also shown in Fig. 9, which indicate the much higher accuracy of the present method over FEM and XFEM. It should be noted, however, that the accuracy of the SIFs is not as high as the HCE method based on truncated asymptotic crack-tip displacement and stress expansions [21] and the hybrid SBFE-FE method using two layers of sub-domains [26], probably due to the displacement discontinuity on the boundary between the SBFE subdomain and the surrounding FE mesh.

The influence of the number of DOFs used to model the SBFE subdomain is shown in Fig. 10. It can be seen that using 30 nodes can achieve an error less than 1\%.

An unstructured mesh with 1652 DOFs shown in Fig. 11a is also used for this example to investigate the effect of the mesh irregularity, as such situations may arise in remeshing. The contour map of the vertical displacement is shown in Fig. 11b. The details around the crack-tip are highlighted in Fig. 11c, showing a good displacement continuity across the FE-SBFE virtual interfaces, as in the structured mesh (Fig. 7b). The computed \( K_I \) is 9.18 with a
2% error. Therefore, the accuracy of the coupled method seems not to be adversely affected by the arrangement of the FE mesh.

5.2. An edge-cracked plate under mixed-mode loading

The second example is an edge-cracked plate which is fixed at the bottom and subjected to a far-field unit shear stress applied on the top, as shown in Fig. 12. The reference solutions are \( K_I = 34.0 \) and \( K_{II} = 4.55 \) [51]. Similar meshes as in the first example are used.

Table 2 compares the computed errors of \( K_I \) and \( K_{II} \) by the FEM [26] and the present method. Fig. 13 shows the convergence of \( K_I \) and \( K_{II} \) with the increasing number of DOFs. As in the first example, the coupled method is more accurate than the conventional FEM for calculating the SIFs with fewer DOFs.

The corresponding crack paths, which are fully automatically predicted by the developed method, are shown in Fig. 14a–c, respectively. It can be seen that the crack paths modelled by different meshes (8 \( \times \) 16, 16 \( \times \) 32, 20 \( \times \) 40 finite elements, respectively) are consistent and in good agreement with those from the FEM-meshless coupling method [10] (see Fig. 14d).

5.3. A single-edge notched shear concrete beam

The third example is a four-point single-edge notched shear concrete beam as shown in Fig. 15, which was first tested and analyzed by Arrea and Ingraffea [51]. It has since become a benchmark for validating mixed-mode crack propagation models [40,43,44,52,53].

The predicted crack propagation process using an initial 21 \( \times \) 42 FE mesh is shown in Fig. 16(a)–(d), which agrees very well with the results obtained from the FEM [40,43,44,53] (see Fig. 19). The final crack paths from 13 \( \times \) 26 and 19 \( \times \) 34 initial FE meshes are shown in Figs. 17 and 18, respectively. The crack paths predicted using all the meshes are close to the ones observed experimentally [51]. The predicted load–crack mouth sliding displacement (F–CMSD) curves are compared with FEM results [44] in Fig. 20. The difference between the peak loads predicted from different meshes is within 2% while the rest parts of the F–CMSD curves virtually coincide. This demonstrates the good mesh objectivity of the developed method.

5.4. A double cantilever beam

The fourth example is a double cantilever beam which is fixed on the right boundary, as shown in Fig. 21 [54]. Fig. 22(a)–(d) show the predicted crack propagation process using a 21 \( \times \) 42 initial mesh. The predicted final crack path looks closer to the experimental observation [54] than other numerical studies [55,56], as shown in Fig. 23.

5.5. A double-edge notched concrete beam

The fifth example is a double-edge notched concrete beam (DEN) subjected to a four-point shear loading, as shown in Fig. 24. The predicted crack propagation process shown in Fig. 25 agrees well with the experimental [57] and other numerical results [40,57].

5.6. A double-edge notched plate with two holes

The last example is a plate with two holes and two edge cracks subjected to a uniform tensile loading, as shown in Fig. 26. Fig. 27(a) and (b) show two final FE–SBFE coupled meshes, with
1722 and 6208 DOFs, respectively. The predicted crack paths using the two meshes are very close to each other. Fig. 28 compares the crack paths predicted by the present method with those obtained by the polygon SBFEM [56] and by the FEM [58].

6. Conclusions

A non-matching finite element-scaled boundary finite element coupled method is developed for modelling crack propagation problems in linear elastic fracture mechanics. The stress singularities are accurately captured by crack-tip SBFE subdomains, making the FE-based remeshing procedure as simple as possible. The use of non-matching FE and SBFE meshes, whose displacement continuity is ensured by assigning sufficiently high stiffness on the virtual interfaces, makes remeshing even more flexible than other methods. The accuracy and the effectiveness of the developed method are demonstrated by modelling a variety of fracture problems. It also paves the way for further development, such as the improvement of the method by a similar technique used in the overlapping methods [34,39,59] in which the cracked subdomain floats on the global FE mesh, namely, the two meshes are completely independent. This will offer the highest flexibility in remeshing procedure.

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References


9.1 Conclusions

The complex crack initiation and propagation process is realistically simulated using the computational technology developed in this study and the numerical results allow better understanding of experimental observations. It is shown how the explicit representation of heterogeneous structures offers interesting prospects for identification, understanding and modelling of macroscopic behaviours. The presented simulations provide valuable insights for quasi-brittle material modelling. The developed computational technology is demonstrated to be an efficient and effective tool for assessment of structural reliability and calculation of material strength and fracture toughness for improved structural design.

The developed cohesive zone model enables simulation of the energy dissipation process in the FPZ during fracture by pre-inserting zero CIEs to the solid elements. It is demonstrated to be an efficient and powerful computational tool that could be easily implemented in modelling quasi-brittle materials. Damage-plasticity model developed for modelling 3D meso-structure of concrete avoids the difficulty of capturing the relation between shear and compressive stress in zero-thickness cohesive zone model, and yields more realistic results in compressive loading conditions. The proposed non-matching SBFE-FE coupled method has been applied to model the LEFM-based crack for the first time. This coupled method is shown to be both theoretically more accurate and numerically more efficient than the formerly used FEM or SBFEM.

The conclusions from the simulations and analysis are summarised as follows:

1. It is found both in 2D and 3D Monte Carlo simulations that the fracture behaviour and stress-displacement responses of the numerical concrete specimens loaded under both uniaxial tension and compression are highly dependent on the random meso-structures, particularly the post-peak softening responses. Therefore, statistical analysis of a sufficient number of samples is necessary for accurate understanding of the peak stress and post-peak responses;
2. Two cracking types are observed for tension tests under the assumed boundary conditions, regardless of the shapes and volume fractions of aggregates and pores/voids, namely: Type I cracking with one dominant macro-crack; and Type II cracking with two or more macro-cracks which shows more progressive post-peak softening;

3. Using polygonal/polyhedral rather than circular/spherical or elliptical/ellipsoidal aggregates, or increasing the aggregate volume fraction reduces the tensile strength of specimens;

4. Void content is found to have adverse effects on the specimen tensile and compressive strength, and thus cannot be neglected in mesoscale fracture modelling of concrete;

5. Numerical results of size effects on 2D heterogeneous concrete show a good agreement with Weibull’s stochastic size effect law; size effect equations for different porosities and aggregate volume fractions are suggested;

6. The third dimension in concrete modelling is demonstrated to have a pronounced influence on both macroscopic mechanical properties and crack patterns in tension. The 3D modelling demonstrates a larger mean peak stress and a smaller standard deviation in the pre-peak response, and a larger standard deviation in the post-peak response, compared to 2D modelling.

9.2 Perspectives

The research work presented in this thesis forms part of computational technology for modelling quasi-brittle materials such as concrete, and a number of promising directions for future research are recommended:

1. More precise calibration of model’s parameters is required in order to correctly reproduce the behaviour of mortar, aggregates and concrete. Additional physical tests for a series of concrete under tension and compression are suggested to be conducted to perform more quantitative comparisons between numerical and experimental results;

2. Although the demonstrations in this study are done for concrete where sufficient data is available for material parameters and result validations, the methods developed are applicable to other quasi-brittle materials, such as high performance concrete, porous concrete, steel reinforced concrete, fibre reinforced composites, graphite,
cement, bones, etc. Thus one of the most significant possible development would be
to extend the proposed computational technology to model a larger class of materials;

3. Development of parallel computing algorithms is desirable to reduce
computational cost and improve efficiency, especially for statistical analysis when a
large number of 3D specimens are used or modelling larger size structures;

4. To accommodate more complex loading conditions and parallel computing, a
user-defined subroutine for cohesive zone modelling with purposely specified
material constitutive laws and criterions of crack initiation is required;

5. Incorporating time dependent phenomena such as aging and creep behaviour,
and coupling process of mechanical, heat transfer, diffusion, would provide further
interesting insight into material’s performance and lead to a wider range of
applicability of the developed computational technology;

6. Extensive statistical analysis based on the 3D images from X-ray tomography,
could lead to a more precise investigation on mechanical behaviour of a variety of
materials. Applying this testing technique would enable a more accurate
representation of the material heterogeneities and direct comparison of micro-cracking
development;

7. Although the FE mesh and SBFE mesh are independent from each other in the
non-matching SBFE-FE method, the size of the SBFE subdomains are dependent on
the shape of the elements around the crack tips. A deeper investigation on the
overlapping SBFE-FE method which focuses on coupling two completely
independent meshes together will offer a highest flexibility in remeshing.

8. Further studies are desirable to consider multi-axial tension and compression,
size effect on 3D, fracture modelling considering rate effects (e.g. seism, blast, shock,
impact, etc.), computational homogenization for effective material properties,
boundary effects on material behaviour, 3D multi-scale (Micro-, meso- to macro-)
fracture simulation of three/four point bending beam, and more complex specimens,
such as cylindrical, panels, notched beams, even structure systems such as nuclear
power plants, dams, etc.