In-situ X-ray Computed Tomography
Characterisation and Mesoscale Image Based
Fracture Modelling of Concrete

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Chapter 1  Introduction ................................................................. 19
  1.1  Background ........................................................................... 19
  1.2  Aims and objectives ............................................................. 21
  1.3  Thesis structure ................................................................. 22

Chapter 2  Literature Review ...................................................... 24
  2.1  Multi-scale modelling .......................................................... 24
  2.2  Numerical characterisation of material heterogeneity ............... 28
  2.3  Non-destructive characterisation of material heterogeneity ........ 31
  2.4  Image-based finite element modelling .................................... 33
  2.5  Numerical modelling of concrete fracture ............................... 34
    2.5.1  The smeared crack models ............................................. 36
    2.5.2  The discrete crack models ............................................. 37
    2.5.3  Cohesive element in ABAQUS ....................................... 43
  2.6  Summary ............................................................................... 48

Chapter 3  In-Situ X-Ray Computed Tomography Experiment ....... 50
## CONTENTS

3.1 X-ray computed tomography ................................................................. 50
   3.1.1 XCT process ................................................................................... 51
   3.1.2 Image reconstruction........................................................................ 52

3.2 Brazilian-like in-situ XCT test ............................................................... 53
   3.2.1 Experiment ...................................................................................... 53
   3.2.2 Reconstruction ................................................................................ 55
   3.2.3 Digital volume correlation .............................................................. 57
   3.2.4 3D segmentation ............................................................................. 58
   3.2.5 Evolution of voids and cracks ......................................................... 65

3.3 Uniaxial compression in-situ XCT test .................................................. 66
   3.3.1 Experiment ...................................................................................... 66
   3.3.2 The damaged sample ...................................................................... 68
   3.3.3 Fracture observed from 2D tomography slices ................................... 69
   3.3.4 Sub-volume micro-cracking ........................................................... 70
   3.3.5 3D segmentation ............................................................................. 72
   3.3.6 Crack propagation in 3D ................................................................. 75
   3.3.7 Evolution of voids and cracks ......................................................... 77
   3.3.8 Crack width and ITZ thickness measurement .................................... 79

3.4 Cyclic compression in-situ XCT test ..................................................... 85
   3.4.1 Experiment ...................................................................................... 85
   3.4.2 Characterisation of fracture features ............................................... 85
   3.4.3 3D segmentation ............................................................................. 90

3.5 Summary ................................................................................................ 94

Chapter 4 Micro-Indentation and Homogenisation ................................. 96

4.1 Micro-indentation test ............................................................................ 96
   4.1.1 Sample preparation ......................................................................... 96
   4.1.2 Micro-indentation test ..................................................................... 97
   4.1.3 Results ........................................................................................... 100

4.2 Homogenisation .................................................................................... 104
   4.2.1 Methodology .................................................................................. 104
   4.2.2 Homogenisation analysis of the 40mm cube ................................... 109
Chapter 5  2D XCT-Image Based Modelling ........................................... 115

5.1 Generation of 2D finite element meshes................................. 115
  5.1.1 Image processing ............................................................. 116
  5.1.2 Initial mesh generation ..................................................... 117
  5.1.3 Insertion of cohesive interface elements ............................. 118

5.2 Model parameters........................................................................ 120

5.3 Typical uniaxial tension results ................................................ 122
  5.3.1 Stress-displacement behaviour ......................................... 122
  5.3.2 Micro-crack propagation ................................................... 123
  5.3.3 Macro-crack propagation ................................................... 125
  5.3.4 Localised fracture ............................................................ 126

5.4 Effects of mesh type and inter-phase boundaries .................... 127

5.5 Effects of loading direction (different micro-structures with the same volume fractions) ......................................................... 129

5.6 Effects of micro-structural heterogeneity .................................. 130

5.7 Crack pattern match of serial slices ......................................... 132

5.8 Statistical analysis of predicted strengths .................................. 133

5.9 Parametric study....................................................................... 135
  5.9.1 Control parameters of the linear cohesive law ....................... 135
  5.9.2 Elastic stiffness of CIEs ..................................................... 138
  5.9.3 Loading magnitude .......................................................... 139
  5.9.4 Boundary condition .......................................................... 139

5.10 Size effect study..................................................................... 140
  5.10.1 Centred meshes with voids .............................................. 140
  5.10.2 Centred meshes without voids .......................................... 144
  5.10.3 Multiple meshes for each size ........................................... 145

5.11 Typical uniaxial compression results ...................................... 147

5.12 Summary................................................................................. 149

Chapter 6  3D XCT-Image Based Modelling ................................. 152

6.1 3D finite element mesh and material parameters ...................... 152
LIST OF FIGURES

Figure 2-1 Multi-length scales for concrete .......................................................... 25
Figure 2-2 Numerical samples with randomised distributions of aggregates and pores (Wang et al., 2015b) ................................................................................. 29
Figure 2-3 A 2D Weibull random sample, with the deep blue areas indicating low tensile strength and the dark red areas representing high tensile strength. The correlation length is 12.5mm and the variance of tensile strength is 0.1 MPa². (Yang et al., 2009) ........................................................................................................... 30
Figure 2-4 Cracking models: (a) Discrete crack; (b) Smeared crack (Kwak and Filippou, 1990) ............................................................................................................. 35
Figure 2-5 T-S curve with linear softening laws (Yang et al., 2009) ..................... 44
Figure 3-1 Illustration of the XCT acquisition and reconstruction processes (Landis et al., 2003) ........................................................................................................... 53
Figure 3-2 The in-situ XCT instrument with DEBEN loading system and a tested specimen. The load was applied by moving the rig upwards, controlled by a computer server system. ................................................................. 54
Figure 3-3 The loading curve of the benchmark in-situ XCT test (Yang et al., 2013) ........................................................ ........................................................ 55
Figure 3-4 Workflow of reconstruction process .................................................. 56
Figure 3-5 Modified force-displacement curve by DVC ..................................... 58
Figure 3-6 AVIZO software interface .................................................................. 59
Figure 3-7 Imported slice views from the 16.5kN dataset ................................... 59
Figure 3-8 Before and after filter operation .......................................................... 60
Figure 3-9 Line-Probe grey values across a xy plane slice ............................... 61
Figure 3-10 Grey-scale-based segmentation result ............................................ 62
Figure 3-11 The segmented binary images: (a) aggregate, (b) voids and (c) cement, black areas represent background ...................................................... 63
Figure 3-12 The 3D views of concrete cube under 16.5kN (loading was under z) .............................................................................................................................. 63
Figure 3-13 The 3D views of concrete cube without load .................................. 64
Figure 3-14 Volume evolution of voids and cracks ............................................ 65
Figure 3-15 The in-situ sample before applying load.................................66
Figure 3-16 The loading history for sample 2...........................................67
Figure 3-17 The modified F-d curve of sample 2 by DVC..........................68
Figure 3-18 The Damaged sample 2 ..........................................................69
Figure 3-19 Propagation of micro-cracks in sample 2, observations from tomography images (xz slice)..............................................................70
Figure 3-20 Sub-volume cracking and localised damage (xz slice).................71
Figure 3-21 3D crack surface and slice views indicating cracks ..................71
Figure 3-22 3D crack surface and slice views at the same location as Figure 3-21 ........................................................................................................72
Figure 3-23 The 3D segmentation of 20mm cube without any load..............73
Figure 3-24 3D volume distribution for aggregates in sample 2 .................74
Figure 3-25 3D volume distribution of voids in sample 2 ............................75
Figure 3-26 Comparison of XCT slice and segmented cracks at 9.1kN load ....76
Figure 3-27 The segmented 3D distribution of voids at 0kN and the propagated crack at each load step (3, 5 and 9.1kN)........................................77
Figure 3-28 Volume evolution of voids and cracks ......................................78
Figure 3-29 The voids and cracks contents along the height direction during loading.........................................................................................78
Figure 3-30 Crack locations ........................................................................80
Figure 3-31 The average grey value distribution of line 1 to 6 in Figure 3-30....80
Figure 3-32 Average curves of grey value distributions for location 1,2 and 3..82
Figure 3-33 The locations of measured ITZ thicknesses ...............................83
Figure 3-34 The average grey value distribution of 20 lines shown in Figure 3-33 ........................................................................................................83
Figure 3-35 Sample 4 before test .................................................................85
Figure 3-36 The loading history of sample 4 .................................................85
Figure 3-37 The damaged sample 4 under cyclic compression ......................86
Figure 3-38 Fracture observed from 2D slices (in xz plane) at different load stages...............................................................................................87
Figure 3-39 Crack network propagation in 3D .............................................88
Figure 3-40 Localised crack features ............................................................89
Figure 3-41 Crack network propagation in a 3D sub-volume ..........................90
Figure 3-42 The 3D segmentation of sample 4 at 0kN ................................91
Figure 3-43 3D volume distribution of aggregates in sample 4 ........................................... 92
Figure 3-44 3D volume distribution of voids in sample 4 .................................................. 93
Figure 4-1 The automatic grinding and polishing machine ................................................. 97
Figure 4-2 Concrete specimens used for the micro-indentation test .................................... 97
Figure 4-3 The CSM micro-indentation tester and its control system ................................. 98
Figure 4-4 Typical indentation force-depth curve ............................................................... 99
Figure 4-5 The force-depth curve and indentation mark of aggregate under 5N ......................... 100
Figure 4-6 The indentation marks of the aggregate under 0.1N ....................................... 101
Figure 4-7 A indentation point near a hole ........................................................................... 101
Figure 4-8 Typical indents for cement and aggregate under 0.3N ..................................... 102
Figure 4-9 Standard force-depth curves for cement and aggregate .................................... 102
Figure 4-10 Periodic body and RVE .................................................................................. 105
Figure 4-11 Reconstructed RVEs with different sizes, with colours in yellow, cyan and purple represent aggregates, cement and voids .................................................. 109
Figure 4-12 Stress distribution of different load cases for RVE10-1 .................................... 110
Figure 5-1 Segmented X-ray tomography of the cube with the matrix in grey, the aggregates in black and the voids in white ................................................................. 116
Figure 5-2 Segmented virtual xy slice (cross-section 1) (a) before and (b) after image processing to improve the FE meshing. The black, grey and white regions represent aggregates, cement and voids, respectively. The insets show magnified regions. ......................................................................................................................... 117
Figure 5-3 The transformation from (a) pixelated image to (b) simple grid and (c) smoothed mesh .......................................................................................................................... 118
Figure 5-4 Insertion of CIEs ............................................................................................. 119
Figure 5-5 The 2D FE mesh for cross section 1 based on the XCT image in Figure 5-2 .................................................................................................................................................. 120
Figure 5-6 Computational cost reduction by parallel processing ....................................... 122
Figure 5-7 σ-d curves under uniaxial tension (volume fractions of aggregates are 52%, 50% and 45% for the present study, experiment (Hordijk, 1992) and reference simulation (López et al., 2008a), respectively) ................................................................................. 123
Figure 5-8 The micro-structure of the reference simulation (López et al., 2008a) ......................................................................................................................................................... 123
Figure 5-9 The evolution of pre-peak micro-cracking for cross-section 1 at various stages in Figure 5-7. (For clarity the 3 phases are not shown.) 125
Figure 5-10 The macro-crack propagation process for cross-section 1 at various stages in Figure 5-7. (The blue, grey, white and red regions represent aggregates, cement, voids and macro-cracks.) 126
Figure 5-11 Sequence showing the cracking propagation leading up to failure for a localised region, $DSF=20$. 127
Figure 5-12 Comparison of mesh types. 128
Figure 5-13 $\sigma$-$\epsilon$ curves predicted from meshes with different element types. 129
Figure 5-14 Crack patterns influenced by element types ($\epsilon=0.0021$). 129
Figure 5-15 Typical crack pattern for cross-section 1 under vertical tension ($\epsilon=0.002$). 130
Figure 5-16 $\sigma$-$\epsilon$ curves under different tension directions. 130
Figure 5-17 Phase volume fractions and predicted tensile strengths for the different cross-sections. 131
Figure 5-18 $\sigma$-$\epsilon$ curves from different images. 132
Figure 5-19 Crack pattern of cross-section 40 ($\epsilon=0.002$). 132
Figure 5-20 Crack pattern of cross-section 100 ($\epsilon=0.002$). 132
Figure 5-21 Crack pattern of cross-section 240 ($\epsilon=0.002$). 132
Figure 5-22 Investigations of serial slices. 133
Figure 5-23 Predicted $\sigma$-$\epsilon$ curves of 372 images in the $yz$ plane and the mean curve. 134
Figure 5-24 The best-fit Gaussian-distribution PDF curve of the predicted strengths. 134
Figure 5-25 The predicted strength and void volume fraction for different slices. 135
Figure 5-26 Effect of cohesive strength and fracture energy on the $\sigma$-$\epsilon$ response. 136
Figure 5-27 Micro-cracks propagated separately ($\epsilon=0.0017$). 137
Figure 5-28 Effects of cement cohesive strength on the crack pattern ($\epsilon=0.0021$ mm). 138
Figure 5-29 The influence of initial stiffness on the $\sigma$-$d$ curve. 139
Figure 5-30 The influence of loading magnitude on $\sigma$-$d$ curve. 139
Figure 5-31 The influence of boundary conditions on the $\sigma$-$d$ curve. 140
Figure 5-32 Mesh locations at different sizes .................................................... 141
Figure 5-33 The $\sigma$-$\varepsilon$ curves for different mesh sizes.............................. 142
Figure 5-34 Crack patterns for different meshes.................................................. 144
Figure 5-35 The $\sigma$-$\varepsilon$ curves for different mesh sizes.............................. 145
Figure 5-36 The predicted average tensile strengths and voids volume fractions
for different meshes ............................................................................................ 146
Figure 5-37 Mean $\sigma$-$\varepsilon$ curves for 10mm, 20mm and 30mm meshes............. 146
Figure 5-38 The predicted average tensile strengths of 10mm, 20mm, 30mm and
37.2mm meshes .................................................................................................. 147
Figure 5-39 The predicted $\sigma$-$\varepsilon$ curves under $X$ and $Y$ compressions .......... 148
Figure 5-40 The crack patterns at maximum load under $X$ and $Y$ compressions
($DSF=10$) ............................................................................................................ 149
Figure 6-1 3D FE meshes of the 40mm benchmark cube and the 20mm cube (Sample 2) .......................................................................................................... 154
Figure 6-2 3D FE meshes of RVE10 and RVE20 cut from 40mm cube .......... 154
Figure 6-3 The CIEs (in red) surrounding aggregate elements in a 10mm cube model.................................................................................................................. 156
Figure 6-4 Boundary conditions of the 40mm cube under the Brazilian-like compression ................................................................. 158
Figure 6-5 Comparison of $F$-$d$ curves from DVC and the 3D FE simulation ....... 158
Figure 6-6 Comparison of crack patterns at peak load ....................................... 160
Figure 6-7 Comparison of crack patterns at post-peak load .............................. 161
Figure 6-8 Damage evolution in the cement and on the interfaces ................. 162
Figure 6-9 Damage propagation with SDEG over 0.99 ($DSF=10$) .................. 163
Figure 6-10 $F$-$d$ curves of 20mm Sample 2 from test and FE simulation........... 164
Figure 6-11 Comparison of damage propagation characterised from the in-situ
XCT tomography images and the FE simulation ................................................. 166
Figure 6-12 Final crack pattern from the in-situ test and the FE simulation ....... 167
Figure 6-13 Stress distribution in the Z direction ($S_{33}$) .................................... 168
Figure 6-14 $\sigma$-$\varepsilon$ curves of the elastic simulation, 2D and 3D fracture modelling simulations ........................................................................................................ 169
Figure 6-15 Comparison of crack patterns of 3D and 2D simulations ($DSF=10$)
............................................................................................................................... 170
Figure 6-16 Internal damage at peak load ($DSF=10$) ....................................... 170
LIST OF FIGURES

Figure 6-17 volumetric average $\sigma$-$\varepsilon$ curves of different volume sizes under compression ....................................................................................................... 171
Figure 6-18 $\sigma$-$\varepsilon$ curves for realisations of RVE10 .................................................. 172
Figure 6-19 $\sigma$-$\varepsilon$ curves for realisations of RVE20 .................................................. 172
Figure 6-20 $\sigma$-$\varepsilon$ curves for benchmark cube under $X/Y/Z$ loads ......................... 172
Figure 6-21 $\sigma$-$\varepsilon$ curves under uniaxial tension (volume fractions of aggregates are 54.8% and 20% for the present sample 2 and the reference (Caballero et al., 2005), respectively) ........................................................................................................... 173
Figure 6-22 The initiation and propagation of micro-cracks ............................................. 174
Figure 6-23 Final macro-crack pattern of sample 2 under tension ......................... 175
Figure 6-24 $\sigma$-$\varepsilon$ curve of RVE10_1 ............................................................................... 176
Figure 6-25 The initiation and propagation of micro- and macro-cracks .............. 177
Figure 6-26 Final cracked surfaces of RVE10 .............................................................. 178
Figure 6-27 $\sigma$-$\varepsilon$ curve in 3D and 2D mean ................................................................. 178
Figure 6-28 Final crack pattern ($DSF=10$) ................................................................. 179
Figure 6-29 Internal 3D crack surfaces ............................................................................. 180
Figure 6-30 $\sigma$-$\varepsilon$ curves of different volume sizes under tension .................. 180
Figure 6-31 $\sigma$-$\varepsilon$ curves for realisations of RVE10 .................................................. 181
Figure 6-32 $\sigma$-$\varepsilon$ curves for realisations of RVE20 .................................................. 181
Figure 6-33 $\sigma$-$\varepsilon$ curves for benchmark cube under $X/Y/Z$ loads ......................... 182
Figure 7-1 Modelling scheme ....................................................................................... 184
LIST OF TABLES

Table 3-1 Volume fraction of each phase in the segmented cube without load ..65
Table 3-2 Volume fraction for each phase in sample 2 ...........................................73
Table 3-3 Statistical analysis for aggregates in sample 2 .......................................74
Table 3-4 Statistical analysis for voids in sample 2 ..............................................75
Table 3-5 Crack widths measured from Figure 3-30 ............................................81
Table 3-6 The measurement of the ITZ thickness at different locations ..............84
Table 3-7 Volume fraction of each phase in sample 4 ...........................................91
Table 3-8 Statistical analysis for aggregates in sample 4 ....................................92
Table 3-9 Statistical analysis for voids in sample 4 ..............................................93
Table 4-1 Estimation of Young’s modulus for aggregate and cement under
different indentation forces ..................................................................................103
Table 4-2 Homogenised engineering constants with associated uncertainties ..112
Table 5-1 Material properties .............................................................................121
Table 5-2 Volume fraction of each phase in different mesh sizes .....................141
Table 5-3 Predicted tensile strength of different meshes under X and Y loads..143
Table 5-4 Volume fraction of each phase in different mesh sizes ....................145
Table 6-1 Volume fraction alteration of the 40mm cube between image model
and the smoothed 3D mesh ..............................................................................153
Table 6-2 Material parameters .........................................................................157
Table 6-3 Comparison of estimated Young’s modulus by different techniques171
This study develops a 3D meso-scale fracture characterisation and modelling framework for better understanding of the failure mechanisms in concrete, by combining in-situ micro-scale X-ray computed tomography (XCT) experiments and XCT image-based finite element (FE) simulations.

Firstly, sophisticated in-situ XCT experiments are conducted on concrete cubes under Brazilian-like, uniaxial and cyclic compression. Proper procedures for XCT image reconstruction and multi-phasic segmentation are identified. The fracture evolution at different loading stages is characterised and visualised as well as the detailed distributions of aggregates and voids. The Young’s moduli of aggregate and cement are obtained by micro-indentation tests and used in XCT-image based asymptotic homogenisation simulations to calculate effective elastic constants of concrete cubes. The XCT technique proves very powerful in characterising and visualising the complicated 3D fracture evolution in concrete.

The material properties and the segmented 3D images from the experiments are then used for FE fracture simulations with realistic aggregates, cement and voids. Image-based mesh generation algorithms are developed for 2D in a MATLAB code and identified for 3D in Simpleware. Cohesive interface elements are embedded within cement and aggregate-cement interfaces to simulate the complex nonlinear fracture. Extensive simulations of 40mm and 20mm cubes under compression and tension are carried out. Good agreements are achieved between the load-displacement curves and final crack patterns from the simulations and those from the compressive in-situ XCT tests. The XCT image-based modelling proves very promising in elucidating fundamental mechanisms of complicated crack initiation and propagation in concrete.
DECLARATION

The University of Manchester

PhD by Candidate Declaration

Candidate Name: Wenyuan Ren

Faculty: Engineering and Physical Sciences

Thesis Title: In-situ X-ray Computed Tomography Characterisation and Mesoscale Image Based Fracture Modelling of Concrete

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# NOMENCLATURE

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### NOMENCLATURE

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<td>4-node bilinear plane stress finite element with reduced integration</td>
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<td>3D</td>
<td>Three-dimension</td>
<td>MRI</td>
<td>Magnetic resonance imaging</td>
</tr>
<tr>
<td>AVG</td>
<td>Average</td>
<td>PDF</td>
<td>Probability density function</td>
</tr>
<tr>
<td>CCM</td>
<td>Cohesive crack model</td>
<td>RVE</td>
<td>Representative volume element</td>
</tr>
<tr>
<td>CIE</td>
<td>Cohesive interface element</td>
<td>SD</td>
<td>Standard deviation</td>
</tr>
<tr>
<td>CIE_AGG</td>
<td>Cohesive interface element inside the aggregates</td>
<td>SDEG</td>
<td>Overall value of the scalar damage variable</td>
</tr>
<tr>
<td>CIE_CEM</td>
<td>Cohesive interface element inside the cement</td>
<td>T-S</td>
<td>traction-separation</td>
</tr>
<tr>
<td>CIE_INT</td>
<td>Cohesive interface element on the aggregate-cement interfaces</td>
<td>US</td>
<td>Ultrasound</td>
</tr>
<tr>
<td>COH2D4</td>
<td>4-node 2D cohesive element</td>
<td>XCT</td>
<td>X-ray Computed Tomography</td>
</tr>
</tbody>
</table>

### Acronyms and Terminology

- **ITZ**: Interfacial transition zones
- **LEFM**: Linear elastic fracture mechanics
- **MRI**: Magnetic resonance imaging
- **PDF**: Probability density function
- **RVE**: Representative volume element
- **SD**: Standard deviation
- **SDEG**: Overall value of the scalar damage variable
- **T-S**: Traction-separation
- **US**: Ultrasound
- **XCT**: X-ray Computed Tomography
Chapter 1

Introduction

This chapter outlines the research background and presents the specific research aims and objectives. It introduces the structure of this thesis and describes how the objectives are accomplished.

1.1 Background

Most materials, if examined at a proper scale (which can range from nano-, micro-, meso- to macro-meters), exhibit heterogeneity and uncertainty (Koutsourelakis, 2006). These include many composite materials, such as concrete, soil, rock, alloys and fibre-reinforced composites, which are widely used in structures for many industries and support a wide range of societal needs. Due to the random distribution of multiple phases, these materials have intrinsically heterogeneous mechanical properties in small-length scales, which in turn directly determine the performance and reliability of structures and systems at large scales. Therefore, understanding their mechanical properties, including damage and fracture at different scales through both experimental studies and computational modelling, becomes an important and challenging engineering and scientific problem (Oden et al., 2003; Kassner et al., 2005; Yang et al., 2009). Such a better understanding of their mechanical behaviour can lead to the development of materials with higher strength, fracture-resistance and durability, more cost-effective manufacturing processes and optimal structural designs, all of which greatly contribute to the economy and sustainability of our society.
Recently, multi-scale experiments and numerical modelling of quasi-brittle multi-phasic materials, such as concrete, have received more and more attention in order to obtain a better understanding of their failure mechanisms (Ren et al., 2015). For both multi-scale modelling and understanding of micro-mechanisms, the internal micro-structure, as well as the in-situ characterisation of damage evolution, is of vital importance, especially for fracture analysis where the phenomena at the local nano- and micro-scales have a significant impact on the failure of structures at the meso- and macro-scales. However, most of the numerical models available in literature use assumed micro-/meso-scale morphologies (Wang et al., 2015b; Yin et al., 2015) or assumed random field properties (Yang et al., 2009; Su et al., 2010b).

More recently, the X-ray Computed Tomography (XCT) technique, routinely used in hospitals for medical diagnoses, is now increasingly becoming an attractive tool for characterising micro-structures of materials, because of its high resolution, non-destructive nature, and clear visualisation in 3D. In the last decade, tremendous efforts have been made in applying the XCT to characterise micro-structures and to study evolutions of damage and fracture for a variety of materials, including geological materials (rock, soil and fossils) (Carlson, 2006), metals and alloys (Babout et al., 2006; Marrow et al., 2006; Qian et al., 2008), porous materials (Kerckhofs et al., 2008), dental composite (Drummond et al., 2005), asphalt mixtures (Masad et al., 2002; Onifade et al., 2013) and concrete (Garboczi, 2002; Wang et al., 2003). However, 3D XCT images have only occasionally been used to build geometrically realistic numerical models to study the mechanical behaviour of materials, for example, by Hollister et al. (Hollister et al., 1994) for trabecular bones, Terada et al. (Terada et al., 1997) for metal matrix composites, Ali et al. (Ali et al., 2009) for carbon/carbon composites, McDonald et al. (McDonald et al., 2011) for foams and Manning et al. for dinosaurs (Manning et al., 2009). In most of these studies, simple linear elastic stress analyses were carried out, or an effective stiffness based on homogenisation method was calculated. Recently, very limited simulations based on XCT images were carried out to model the crack opening and fracture process zone in poly-granular graphite (Mostafavi et al., 2013a) and interfacial damage.
in carbon/carbon composites (Sharma et al., 2012). However, the fracture of materials with complex micro-structures such as concrete based on realistic micro-structures has received little attention. Exceptions include recent in-situ micro-XCT image based two-dimension (2D) FE studies using the cohesive crack model (Ren et al., 2015) and 3D studies using the concrete damage plasticity model (Huang et al., 2015).

Numerical modelling of fracture in concrete has been actively conducted since the 1960s (Clough, 1962; Ngo and Scordelis, 1967; Nilson, 1968). In comparison with other modelling techniques, it appears that the discrete crack models, mostly based on the cohesive crack model (CCM), are used extensively, because of their ability to model cracks with strong discontinuities (Su et al., 2010a; Verhoosel et al., 2010) and the ease of their implementation in finite element analysis (Yang et al., 2009; Su et al., 2010b; Yin et al., 2013). However, 3D image-based modelling of complex discrete cohesive crack initiation and propagation in concrete has not been conducted, to the best knowledge of the author.

1.2 Aims and objectives

This research aims to characterise the internal micro-structure and the damage evolution process of concrete specimens, using the state-of-the-art in-situ XCT experimental technique, and also to develop and validate XCT-image based finite element (FE) models with realistic micro-structures for complex meso-scale fracture modelling in concrete. Complicated 2D and 3D crack propagation will be modelled by embedding cohesive interface elements into FE meshes. The numerical models will be calibrated and directly validated against the in-situ XCT tests and micro-indentation tests.

The specific objectives are:
(1) To analyse the benchmark in-situ XCT test of a 40 mm concrete cube, and to set up a standard procedure of image reconstruction, segmentation and post processing;
Chapter 1 Introduction

(2) To characterise the detailed fracture behaviour, and to obtain a better understanding of the fundamental fracture mechanisms, by analysing the in-situ XCT images of the concrete specimens and sub-volumes;
(3) To statistically analyse the concrete cubes and to give recommendations for generating micro-structures;
(4) To develop high-fidelity computer algorithms for transforming 2D and 3D micro-scale XCT images into meso-scale FE meshes consisting of various solid elements, cohesive interface elements and voids;
(5) To develop FE models capable of simulating complex 2D and 3D damage and fracture processes in the concrete specimens;
(6) To directly validate the 3D FE simulations of complex damage and fracture patterns with in-situ XCT images.

1.3 Thesis structure

This thesis contains seven chapters and is structured as follows:

Chapter 1 briefly presents the research background, the research aim and objectives, and the structure of the thesis.

Chapter 2 reviews the literature on multi-scale modelling; numerical and non-destructive experimental characterisation of material heterogeneity; the state-of-the-art image based modelling; and fracture modelling methods for concrete with an emphasis on the cohesive crack model.

Chapter 3 presents the in-situ XCT experiments, including an introduction to the XCT technique, Brazilian-like compression tests of 40mm cubes, and uniaxial and cyclic compression tests of 20mm cubes. The XCT experimental procedure, image processing and segmentation, characterised fracture features and statistical analyses of distributions of aggregates and voids, are presented in detail.

Chapter 4 introduces two techniques that are used: the micro-indentation test for estimation of Young’s moduli of aggregates and cement, which are used as
material parameters for later image-based modelling; and the homogenisation method to calculate the effective elastic modulus of the concrete cube, which is used to validate the elastic behaviour of FE simulation results.

Chapter 5 presents the development of 2D XCT image-based FE models and the main numerical results of concrete cubes under compression and tension. The algorithm of automatically converting XCT images into FE meshes is discussed in detail.

Chapter 6 presents the developed 3D XCT image-based FE models of concrete cubes. The FE models are validated against the in-situ XCT tests of two concrete cubes under the Brazilian-like compression and uniaxial compression, respectively.

Chapter 7 draws the main conclusions from the results of the work and outlines a few suggestions for future work.
THIS chapter reviews several key aspects to accomplish the research aim and objectives set out in Chapter 1, including multi-scale modelling; numerical and non-destructive experimental characterisation of material heterogeneity; state-of-the-art image based modelling; fracture models of concrete, mainly the cohesive crack model that is used in this study. As a vast amount of knowledge exists, the current review is limited to quasi-brittle cement based composites, such as concrete. The merits of different numerical and experimental models and methods are discussed, leading to the selection of X-ray computed tomography (XCT) for characterisation, and pre-inserted cohesive interface elements for fracture modelling.

2.1 Multi-scale modelling

Most materials exhibit inherent heterogeneity and randomness when they are examined at small scales, from nano-, micro- to meso-meters (Koutsourelakis, 2006). These include a wide range of engineering materials, such as rocks and soils in geotechnical engineering, concrete and fibre reinforced concrete in civil engineering, alloys and fibre reinforced polymers in aerospace structures. Figure 2-1 illustrates the multi-length scales for concrete.
Random heterogeneous composite materials usually consist of two or more phases randomly distributed throughout the volume. These phases have different physical or mechanical properties. Naturally, the heterogeneity and randomness of the multi-phases in turn directly determines the performance and reliability of the composites and even the structural systems. Therefore, understanding their mechanical properties, including damage and fracture at different scales, through both experimental studies and computational modelling, becomes a critical and challenging engineering and scientific problem (Oden et al., 2003; Kassner et al., 2005; Ren et al., 2015).

There exist many challenges in multi-scale modelling of heterogeneous composites, for example, the lack of accurate understanding of fundamental 3D deformation mechanisms at multiple scales, particularly at micro- and nano-scales due to limitations of experimental techniques, and the missing links between the scales (Graham-Brady et al., 2006). In order to develop accurate multi-scale models capable of characterising appropriate material behaviour, the intrinsical uncertainties at all scales must be investigated as well. But how to quantify the uncertainties caused by heterogeneous properties remains a challenge.
Compared with routine FE modelling of macro-scale structures assuming homogeneous material behaviour, heterogeneous modelling at smaller length scales (meso-, micro- and nano-scale) is much more challenging, both in building physically-based high-fidelity models and in solving very large equation systems often with millions of degrees of freedom that even supercomputers struggle to tackle. The computational cost may soar even further beyond the computational power of the supercomputers, when the physical behaviour to be modelled is strongly nonlinear, for example, fracture and damage evolution involving material softening which is the topic of this research project.

In order to reduce computational cost in modelling heterogeneous materials at small length scales, many effective media theories have been developed (Hashin and Shtrikman, 1963; Hill, 1963; Milton, 2002; Xu and Graham-Brady, 2005) but they are mostly limited in obtaining the effective properties at a large length scale. More sophisticated multi-scale methods are gradually becoming efficient and exhibiting improved performance, especially in predicting localized phenomena such as damage and fracture (Hughes et al., 1998; Samaey et al., 2005; Koutsourelakis, 2006; Sun et al., 2013).

Conceptually, multi-scale methods can be grouped into two categories: concurrent and hierarchical (Liu et al., 2004). Concurrent methods simultaneously solve a fine-scale model in some local regions of interest and a coarser-scale model in other regions (Oden et al., 2006). For systems whose behaviour at one scale depends strongly on that at another scale, concurrent approaches are usually required. Lu et al. (Lu et al., 2006) presented a concurrent multi-scale modelling approach that couples quantum-mechanical, classical atomistic and continuum mechanical simulations in a unified fashion. Hierarchical, or serial coupling methods (E et al., 2007), use results of a fine-scale model to acquire data for a coarser-scale model that is used globally. The sequential ones are effective in systems where the different scales are weakly coupled. Difficulties typically arise from modelling defects in atomic lattices, dislocations and failure phenomena. From a numerical viewpoint, the two categories are very much related. For both methods, the key numerical aspect is
to design fine-scale simulations that would provide data for coarse-scale models. In addition, the results of a concurrent simulation can be used to determine the system constitutive relationships, which is useful for the hierarchical method. Therefore, the two strategies can be used together to yield optimal efficiency.

One of the main challenges for all multi-scale methods is passing information between the different length scales of the problem. This issue is even more severe for stochastic analyses (Graham-Brady et al., 2006). Three aspects should be paid special attention to, with respect to the passing of information between scales, namely: quantifying the error associated with each length scale; proof of convergence; physical and model uncertainty (Xu and Graham-Brady, 2005; Graham-Brady et al., 2006; Xu and Chen, 2009; Xu, 2014).

Haidar et al. (Haidar et al., 2003) applied a simplified computational technique based on a refined global-local method to investigate the failure of concrete structures. This method comprises two parts: a linear elastic analysis on a coarse mesh over the entire structure; and a non-linear analysis over a small part of the structure near the crack zone, modelled by a dense FE mesh. These two computations are coupled iteratively. Yet, except for some computational weaknesses, there are specific requirements which need to be fulfilled regarding the global and local length scales.

Homogenisation-based multi-scale modelling has also been a topic of extensive research. Of crucial importance is the existence of the representative volume element (RVE) for softening materials. Briefly speaking, a microscopic sample is considered to be an RVE when (1) an increase in its size does not lead to considerable differences in the homogenised properties; (2) the microscopic sample is large enough so that the homogenised properties are independent of the micro-structural randomness. However, this is still being debated in the literature. On one hand, Gitman et al. (Gitman et al., 2007) showed that RVE cannot be found for softening materials, since the material loses statistical homogeneity upon strain localization. On the other hand, Nguyen et al. (Phu Nguyen et al., 2010) proposed a numerical demonstration of the existence of RVE for a class of
softening materials with a random micro-structure such as concrete. Verhoosel et al (Verhoosel et al., 2010) also proved the existence for softening materials, by deriving a traction-separation law (for a macro-crack) instead of a stress-strain relation from the microscopic stresses and strains, as is usually done in standard computational homogenisation schemes.

As aforementioned, either from the deformation mechanism or multi-scale modelling point of view, the micro information is of crucial importance and directly relates to localised behaviour, especially for fracture analysis where the phenomena at the local nano- and micro- scales have a significant impact on the failure of structures at the meso- and macro-scales. Fairly recently, significant discussion has been centred on the role of imaging technologies (Drummond et al., 2005; Withers et al., 2012; Maire and Withers, 2014). With available 2D and 3D imaging technologies, there is an ability to measure geometry, at essentially any length scale, which provides the possibility to experimentally observe the in-situ fracture behaviour at a very fine scale, and then build realistic meshes for later simulation applications.

### 2.2 Numerical characterisation of material heterogeneity

Basically, there exist two types of numerical approaches to characterise the random heterogeneity in materials: direct approaches and indirect approaches (Lilliu and van Mier, 2003; Yang et al., 2009; Su et al., 2010b; Yin et al., 2013; Ren et al., 2015). In the direct approaches, different phases including the matrix, inclusions and interfaces are explicitly modelled by finite elements, each with specific properties. The randomness in the spatial distribution of different phases is realised by randomised positions and shapes of inclusions (e.g., aggregates, fibres, and pores). In the indirect approaches, the material properties, such as the tensile strength and the fracture energy, are modelled as spatially-varying random fields with given correlation structures in the domain of interest so that different phases are implicitly modelled.
Both the direct and the indirect approaches have been widely employed. As examples of the direct approaches, Zhu et al. (2004), Teng et al. (2004) and Lopez et al. (2008a; 2008b) explicitly modelled the matrix, coarse aggregates and interfaces, as random shapes and sizes in concrete specimens under tension and compression, but limited to 2D. Realistic and complex crack patterns were successfully simulated. By using a similar approach, Caballero et al. (2006) extended their 2D model into 3D, and successfully modelled 3D meso-scale fracture in an 80 mm concrete cube with 14 and 64 randomly distributed aggregates explicitly embedded in the matrix. Trias et al. (2006) explicitly modelled fibres as plane circles in 2D RVEs of carbon fibre reinforced polymers. Al-Ostaz et al. (2007) carried out a similar study using Voronoi cells and Delaunay triangulation to characterise random distribution of fibres in a polymer matrix. Wang et al. (2015b) randomised shape, size, volume fraction and spatial distribution of aggregates and pores within 2D concrete samples (see an example of numerical samples in Figure 2-2). Extensive simulations under uniaxial tension were carried out to investigate multiple features related to the fracture pattern and the load-displacement curve as well as size effects (Wang et al., 2015a).

Figure 2-2 Numerical samples with randomised distributions of aggregates and pores (Wang et al., 2015b)
In the indirect approaches, many methods have been developed for generating realistic random fields of material properties (Xu and Graham-Brady, 2005; Koutsourelakis, 2006). However, most of them have not been used in damage and fracture modelling. By modelling material properties as non-Gaussian random fields (typically a Weibull distribution for concrete), Yang and Xu (Yang and Xu, 2008), Bruggi et al. (2008) and Most and Bucher (2007) modelled discrete crack propagation in concrete beams. The Weibull integral method proposed by (Bazânt and Planas, 1998) is able to take into account the random heterogeneity of material strength, but it does not require a large number of random samples. It was recently generalised to model structures with non-uniform stress fields (Bažant et al., 2007) and applied to size effect investigations (Vořechovský and Sadílek, 2008). Although it is simple and efficient, this method has limitations. For example, it can neither consider spatial correlation of local strengths, nor explicitly model crack initiation and propagation processes. Yang et al. (2009) further combined Weibull random fields, to represent spatial distribution of material properties, and Monte Carlo simulations, to evaluate statistical information of structural responses. Figure 2-3 shows a typical Weibull random sample.

![A 2D Weibull random sample, with the deep blue areas indicating low tensile strength and the dark red areas representing high tensile strength. The correlation length is 12.5mm and the variance of tensile strength is 0.1 MPa$^2$.](Yang et al., 2009)
However, most of these numerical models use assumed micro-/meso-scale morphologies or assumed random field properties, rather than using direct and accurate representations of the internal structures of the materials. Therefore, the simulated micro-/meso-scale damage and fracture processes cannot be directly and accurately validated, although macro-scale load-displacement curves can be compared with experimental results.

2.3 Non-destructive characterisation of material heterogeneity

Many experimental techniques exist for non-destructive characterisation of material heterogeneity. Only three commonly used ones are reviewed here: ultrasound (US), magnetic resonance imaging (MRI) and XCT.

The US is used extensively for clinical applications, such as real-time imaging of muscles, tendons, fascia, blood vessels and other soft tissues (Sikdar et al., 2009). The velocity and attenuation of ultrasonic waves propagating through a sample provide information of the physical properties, such as composition, texture, density and rheology. Nowadays, advanced US methods have also been applied to engineering applications. Hernandez et al. (2006) applied US to estimating the porosity in the mortar. Punurai et al. (2007) used direct ultrasonic attenuation to measure the volume fraction and average size of entrained air voids in hardened cement paste samples. Aggelis and Shiotani (2008) carried out simple through-transmission measurement, to examine the influence of concrete inhomogeneity on the attenuation of ultrasound. Chai et al. (2011) discussed tomographic reconstruction using US attenuation for concrete. Although being safe, fast and cost-effective, the US tests are mostly used to non-destructively inspect flaws and remotely measure objects.

The MRI is another well-established non-destructive technique capable of acquiring internal structures of composites (Defraeye et al., 2013). MRI has the following features: (1) it is non-intrusive, which allows monitoring of intact samples over time; (2) 3D spatial information on the internal structure is obtained; (3) different parameters, related to the micro-structures, can be measured, which
often provide complementary information; (4) different phases can be distinguished. The use of MRI dates back to early 1997, when Clark et al. (1997) applied MRI to pre- and post-harvest studies of fruits and vegetables. This technique showed a great ability to provide highly resolved spatial information concerning the distribution and magnetic environment of water in soft tissues. Defraeye et al. (2013) focused attention on MRI for tissue characterisation, with respect to inner and outer cortex tissue, fertilisation treatment, storage time and internal browning. It has been proved that MRI can also be applied to material science as well as medical diagnostics (diagnosis of human diseases like cancer) and biochemical research. Pomerantz et al. (2008) performed MRI measurements of porosity and relaxation time on a series of sandstone and carbonate rock cores to assess spatial heterogeneity in these samples. Wolter (2010) reviewed the applications of MRI for non-destructive measurement of moisture-related properties in concrete. Despite the broad potential use of MRI for characterising materials, such as determination of moisture content profiles, liquid transport coefficients and early-age hardening in concrete, it would be difficult to prove its cost-effectiveness; and furthermore ferromagnetic reinforcement in materials (e.g. steel bars in concrete) would sometimes cause problems (Wolter, 2010). In fact, any materials that didn’t contain water (e.g. metals) cannot be imaged by MRI.

The XCT is another powerful non-invasive 3D imaging technique, which is routinely used in hospitals for the imaging of surface and deep structures within the human body. It has recently been introduced into material science, and has become a powerful imaging technique for characterising the micro-structures of materials (Salvo et al., 2003). Basically, XCT uses X-rays to produce tomographic images of specific areas of a scanned object, allowing the user to visualise the interior of the object without cutting. In the last decade, tremendous efforts have been made in applying XCT to characterise micro-structures and to study evolution of damage for a variety of materials, including trabecular bones (Hollister et al., 1994), dinosaurs (Manning et al., 2009), geological materials (rock, soil and fossils) (Carlson, 2006; Gao et al., 2012), metals and alloys (Terada et al., 1997; Babout et al., 2006; Marrow et al., 2006; Qian et al., 2008), porous materials (Kerckhofs et al., 2008; McDonald et al., 2011), dental
composite of Restolux (Drummond et al., 2005), carbon/carbon composite (Ali et al., 2009; Sharma et al., 2013a), asphalt mixtures (Masad et al., 2002; You et al., 2009; Onifade et al., 2013) and concrete (Garboczi, 2002; Wang et al., 2003). This technique provides a direct way of gaining an insight into the interaction between damage mechanisms and micro-structures.

However, most existing XCT studies have only examined the internal structures of intact materials without external loading, or damaged materials after loading (i.e. post-mortem studies). In-situ XCT studies, which scan the internal structures of materials under progressive loading, so that structural damage and fracture evolution can be examined and related to the loading process, are still rare (McDonald et al., 2011; Mostafavi et al., 2013b; Yang et al., 2013).

### 2.4 Image-based finite element modelling

The recently developed image-based modelling (IBM) techniques (Yue et al., 2003; Ali et al., 2009; Michailidis et al., 2010; Sharma et al., 2012; Petit et al., 2013; Sharma et al., 2014; Huang et al., 2015; Ren et al., 2015) enable precise FE simulations of realistic material micro-structures. High-resolution cameras (Yue et al., 2003) and XCT scanners (Pistoia et al., 2002; Ren et al., 2015; Sui et al., 2015) can be used to capture 2D and 3D images of specimens. The images are then reconstructed and transformed into FE meshes modelling the original micro-structures including realistic shape, size and distribution of each phase. The image-based models can help engineers to optimise the micro-structures of a material for user-specified properties without the need of complex experimental tests. This could be particularly useful in the case of multi-axial loading, which is not easy to carry out experimentally.

In terms of 3D image-based mesh generation, there are broadly two categories: the surface-based meshing approach and the voxel-based meshing approach. For the surface-based approach, surfaces of inclusions such as aggregates in concrete are first extracted from image data and further simplified when necessary; the resultant geometric model is then meshed using sophisticated mesh generation
algorithms. Significant user interactions with manual operations are often involved, such as CAD-based meshing (Wirtz et al., 2003), and the geometric model may be over-simplified, resulting in loss of accuracy (Antiga et al., 2002). The voxel-based meshing approach appears more straightforward: (Yue et al., 2003; Young et al., 2008; Huang et al., 2015), in which each voxel (or pixel in 2D) in an image is directly converted into a same-sized FE element. In this way, the complicated morphologies of multi-phases in the image are retained. However, the interfaces between phases are zigzagged, which may lead to spurious stress concentration and thus high computational costs.

Recently, as the development of imaging technique and its broad applications on material science, several commercial software packages have been developed, such as AVIZO (AVIZO, 2013) and Simpleware (Simpleware, 2011), by which the image models can be segmented and exported as 3D FE meshes. However, considerable user interaction and simplifications are still needed to generate desired meshes, especially for complicated multi-phasic composites like concrete. Developing source codes for advanced research is still much needed.

2.5 Numerical modelling of concrete fracture

As typical quasi-brittle materials, cement based composites are widely used for making architectural structures, foundations, brick/block walls, pavements, bridges, roads, dams, etc. (Jaiswal et al., 2014). Cement based materials exhibit a large number of micro-cracks, especially, at the interfaces between inclusions and the matrix, even before they are subjected to any load. The presence of these micro-cracks has a great effect on mechanical behaviour, since the crack propagation during loading contributes to the nonlinear behaviour at low stress levels, and causes volume expansion near failure (Taqieddin, 2008). Many of these micro-cracks are caused by segregation, shrinkage or thermal expansion of the matrix. Some micro-cracks may develop during loading because of the difference in stiffness between the inclusions and the matrix. Since the inclusion-matrix interface normally has a significantly lower tensile strength, it constitutes the weakest link in the composite system. This is the primary reason for the low
tensile strength of this kind of cement based composite. Taking concrete as an example, the damage may be either at micro-scale or macro-scale. At the micro-scale level, damage is the accumulation of micro-stresses in the neighbourhood of the defects, or interfaces, and the breaking of bond between aggregate and cement (Huang, 2004). At the macro-scale level, damage is the growth of micro-damage into visible cracks. Macro-damage is studied through fracture mechanics, with the variables defined at the macro-scale level. Micro-damage may be studied through the damage variables at a micro-scale level, in which micromechanics are used.

Numerical modelling of crack propagation in concrete has been an active research field since the 1960s (Ngo and Scordelis, 1967). Nowadays, there exist a large number of numerical methods. In terms of how the cracks are modelled geometrically, there are basically two kinds of crack models (Chen, 2010): smeared crack models which treat concrete as a continuum and capture the deterioration process in cracked concrete through a constitutive relationship; and discrete crack models, which explicitly separate crack surfaces to model discontinuity, as shown in Figure 2-4. In the following sections, these methods are elaborated.

Figure 2-4 Cracking models: (a) Discrete crack; (b) Smeared crack (Kwak and Filippou, 1990)
2.5.1 The smeared crack models

In the smeared crack models, the fracture is represented in a smeared manner (see Figure 2-4b), many finely spaced cracks are distributed (smeared) perpendicular to the principal stress direction over the finite element (Rashid, 1968; Bazant and Planas, 1997; Gálvez et al., 2013). The cracks are usually modelled by changing the constitutive (stress-strain) relations of the material in the vicinity of the crack. The constitutive laws defined by stress-strain relations are non-linear and have a strain softening.

Smeared crack models may be categorised into two groups: the fixed smeared crack model (Rashid, 1968; Suidan and Schnobrich, 1973) and the rotating smeared crack model (Gupta and Akbar, 1984; Willam et al., 1987). They differ in the assumption made for the direction of crack propagation (Rots and Blaauwendraad, 1989): with the fixed concept, the orientation of the crack is fixed during the entire computational process, whereas the rotating concept allows the orientation of the crack to co-rotate with the axes of principal strain.

The earliest procedure involved dropping the material stiffness to zero in the direction of the principal tensile stress, when the calculated stress exceeded the tensile capacity of the concrete (Bazant and Planas, 1997). Simultaneously, the stresses in the concrete were released and reapplied to the structure as residual loads. Models of this type exhibit a system of distributed or smeared cracks. Ideally, smeared crack models should be capable of representing the propagation of a single crack, as well as a system of distributed cracks, with reasonable accuracy.

A number of numerical and practical problems occurred with the application of smeared crack models. The principal problem involves the phenomenon of strain localization. When micro-cracks form, they often tend to grow non-uniformly into a narrow band (called a crack). Under these conditions, deformation is concentrated in a narrow band, while the rest of the structure experiences much smaller strains. Because the band of localized strain may be so narrow that conventional continuum mechanics no longer applies, various localization
limiters have been developed, such as gradient models (Schreyer, 1990), the crack band model (Bazânt and Planas, 1998), and the non-local continuum model (Bazant and Planas, 1997). These localization limiters are designed to deal with problems associated with crack localization and spurious mesh sensitivity, that are inherent in softening models in general and for smeared cracking in particular.

Recently, Chen et al. (2012) conducted a number of studies on the shear strengthening of reinforced concrete beams with externally bonded fibre-reinforced polymer reinforcement in the form of strips, plates or sheets. They adopted the crack band model, which relates the element size to the constitutive law of the concrete, so that the fracture energy is independent of element size. It has been shown, by Bazant and Planas (1998), that the smeared crack model yields approximately the same results as the discrete crack model, when the crack band model is employed taking the crack opening displacement \( w \) as the cracking strain \( \epsilon_{cr} \) accumulated over the width \( h_c \) of the crack band in a smeared crack model:

\[
  w = \int_{h_c} \epsilon_{cr} dh
\]  

(2-1)

However, it is difficult for existing smeared crack models to simulate macroscopic discrete cracks and particularly to calculate crack widths. (Yang et al., 2009).

### 2.5.2 The discrete crack models

#### Historical development

Finite element analysis was first applied to the cracking of concrete structures by Clough (1962), Ngo and Scordelis (1967), and Nilson (1968). Ngo and Scordelis (1967) modelled discrete cracks, by separating the nodal points of the finite element mesh and thus creating a discrete crack model (as shown in Figure 2-4a). But they did not address the problem of crack propagation. Nilson (1968) modelled progressive discrete cracking, using a strength-based criterion rather than fracture mechanics techniques. The stress singularity that occurs at the crack
Chapter 2 Literature Review

tip was not modelled. Thus, since the maximum calculated stress near the tip of a crack depends upon element size, the results were mesh-dependent (non-objective).

Linear elastic fracture mechanics (LEFM) is the basic theory of fracture, which was introduced by Griffith (1921) and completed by Irwin (1957) and Rice (1968). LEFM is based on an ideal situation in which the material is elastic except in a vanishing region, which is the crack tip. This concept can be applied to describe the behaviour of any material with cracks, if the size of the inelastic zone is small compared to the dimension of the elastic domain.

Kaplan (1961) seems to have been the first to have performed physical experiments regarding the fracture mechanics of concrete structures. He applied the Griffith (1921) fracture theory (later developed to be LEFM) to evaluate experiments on concrete beams with notches. Kaplan concluded, with some reservations, that the Griffith concept (of a critical potential energy release rate, or critical stress intensity factor, being a condition for crack propagation) is applicable to concrete.

In 1976, Hillerborg et al. (1976) studied the fracture process zone in front of a crack in a concrete structure, and found that it is long and narrow. This led to the development of the fictitious crack model, which is probably one of the simplest nonlinear discrete fracture mechanics models applicable to concrete structures. He introduced the concept of fracture energy (total surface energy required to completely separate the interface at a given point) and the critical stress (the crack tip stress value from which the crack is assumed to propagate), that are parameters in the cohesive force versus crack opening relationship. A large number of cohesive models have subsequently been developed, with a wide range of applications.

The fictitious crack model has proved to be suitable for this purpose, as concrete is a micro-cracking material with a stress-strain curve which may, as a rule, be assumed to be linear all the way up to the peak (Hillerborg, 1991). The size of
the fracture process zone for concrete is often of the order of 100 mm at maximum load on a structure (Bazant and Planas, 1997), which makes LEFM unsuitable for normal structural sizes. The possibility to analyse, not only the propagation of cracks, but also the formation of cracks in an un-cracked structure, also makes the fictitious crack model superior to LEFM for practical applications (e.g. fracture analyses of concrete structures).

When the discrete crack model is implemented in an FE analysis, the cracks are commonly defined along element boundaries. This inevitably introduces a mesh bias (Borst et al., 2004). Automatic re-meshing algorithms (Ingraffea and Saouma, 1985; Yang et al., 2003; Yang and Chen, 2004; Yang and Chen, 2005) were thus developed to solve this mesh bias. However, overcoming computational difficulties associated with topology changes due to re-meshing remains a challenge (Chen et al., 2012). A more detailed review of the discrete cohesive crack model, which will be used in the following chapters, is presented in the following sections.

Cohesive crack model

It appears now that the discrete crack models, mostly based on the cohesive crack model (CCM) developed in ductile materials by Barenblatt (1959) and Dugdale (1960) and in quasi-brittle materials by Hillerborg (1976), are becoming more and more popular. This is because of their ability to model macroscopic cracks with strong discontinuities, the CCM’s capability of realistically representing the energy dissipation during the fracture processes, and the ease of implementation as cohesive interface elements (CIE) in FE Modelling (Yang et al., 2009; Su et al., 2010b).

Needleman (1987) was one of the first to use polynomial and exponential types of traction-separation (T-S) equations to simulate inclusion debonding in metal matrices. He suggested that for inclusions, sufficiently small with respect to a characteristic length, decohesion occurs in a ductile fashion, whereas for sufficiently large inclusions, de-cohesion occurs in a brittle manner. He and Xu (1994; 1995) later developed a potential-based model incorporating both normal
and tangential T-S relationships. This model is widely used since then, due to its simplicity.

Tvergaard (1990; 1995) investigated debonding behaviour at the fibre-matrix interface using CCM with both normal and tangential separations. Geubelle and Baylor (1998) utilized a simple CCM with a linear softening branch, to simulate spontaneous initiation and propagation of transverse matrix cracks and delamination fronts in thin composite plates subjected to low-velocity impact. Elices et al. (2002) validated the CCM predictions for concrete and different notched samples of a glassy polymer and some steels. Zhang and Paulino (2005) investigated dynamic failure processes in homogeneous and functionally graded materials. Alfano and Sacco (2006) further combined interface damage and friction in the CCM by assuming the friction occurs only on the fully damaged part. Song et al. (2006) used CCM to predict the mixed-mode crack trajectory, and found it was in close agreement with experimental results. Yang et al. (2009) analysed crack propagation in concrete with its random heterogeneity by pre-inserting CIEs. Barani et al. (2011) employed the zero-thickness CIE for the mixed mode fracture behaviour of concrete gravity dams. Aragão et al. (2011) introduced a micro-mechanical cohesive model for heterogeneous asphalt concrete mixtures. Yin et al. (Yin et al., 2015) embedded CIEs into random heterogeneous asphalt mixture to conduct tensile fracture simulations. Wang et al. (Wang et al., 2015b) further extended the method of embedding CIEs in random numerical models, by considering the shape, size, spatial distribution of aggregates and the effect of voids. Ren et al. (Ren et al., 2015) developed 2D meso-scale FE models with realistic micro-structures. The CIEs were pre-embedded to simulate complex crack propagation process.

Generally, two types of approach are used to model cohesive crack propagation. The first approach is based on sophisticated remeshing procedures that constantly modify the mesh as cracks propagate (Wawrzynek and Ingraffea, 1989; Yang and Chen, 2004). For problems with unknown crack paths, the interface elements are automatically inserted into the finite element mesh according to a remeshing algorithm when an objective crack propagation criterion is matched. The
calculations of stress intensity factors and stresses at crack tips are usually required. The very fine meshes near crack-tip are often used to guarantee the accuracy. The simulations involving remeshing also suffer from very slow convergence rate, especially on approaching the peak load and in the post-peak phase. This in turn exacerbates the complexity of the remeshing procedure. Besides, the remeshing-based approaches often have difficulties to deal with multiple cracking and 3D problems. The applications of the remeshing-based approaches have been largely limited to 2D fracture problems with a single or a few cracks, although being computationally efficient because a relatively small number of nonlinear CIEs are required in the meshes. The CIEs can also be dynamically inserted when a certain crack initiation criterion is satisfied (Pandolfi and Ortiz, 2002), so that the number of CIEs varies with the loading and the total number of CIEs remains relatively low. These procedures of dynamically inserting CIEs need objective crack initiation criteria and change meshes.

In another approach, CIEs are pre-inserted between the finite elements in the initial meshes (Yang et al., 2009; Su et al., 2010b; Huang et al., 2015; Ren et al., 2015; Wang et al., 2015b). Crack propagation is modelled by automatic opening, bridging, merging and closing of the CIEs under applied loadings. No complex remeshing procedures or explicit fracture criteria are needed. However, these approaches limit the cracks to the finite element boundaries or surfaces, and the predicted crack patterns may thus be mesh-dependent. Another disadvantage is the high computational cost due to the use of a large number of non-linear CIEs.

As an alternative and well-established way to model crack development in composite materials, the CCM has received increasing attention (Yang and Xu, 2008; Kim, 2011). The advantages are: 1) It removes the stress singularity at the crack tip; 2) It provides an efficient tool that can be easily implemented in various computational methods, such as finite element and discrete element methods; 3) it can model both brittle and ductile fracture.
Although being simple and easy to implement, using CCM may eventually become computationally expensive. Because many cohesive elements need to be inserted a priori within the FE mesh. Thus, the potential crack paths are limited by the topology of the FE discretisation. This mesh-dependence problem has been reported (Xu and Needleman, 1994; Scheider and Brocks, 2003). This problem can evidently be controlled by the generation of very highly refined meshes. Another problem associated with the inherent artificial compliance of CCM, (caused by the assumption of initial stiffness) is the displacement discontinuities in the un-cracked parts when external loads are applied (Camacho and Ortiz, 1996; Kim, 2011). However, this problem may be effectively dominated by specifying very high values of initial stiffness in the CCM (Geubelle and Baylor, 1998; Zhang and Paulino, 2005; López et al., 2008a; Ren et al., 2015; Wang et al., 2015b).

**Recent developments**

The prediction results of fracture simulations are highly reliant on the parameters used in the T-S law. Recently, researches have been conducted, by either improving the determination methods for these parameters, or developing new CCM laws by adding and/or changing parameters in the initial T-S curve.

Some of the examples are: Ye and Chen (2011) proposed a micro-mechanical model, based on the periodic representative volume element (RVE) technique, to predict the cohesive strength for numerically simulating composite delamination. Chen et al. (2013) chose CCM parameters by matching simulation predictions with experimental data for the load-crack extension curve of a Mode I stable tearing crack growth event, which are also used for mixed-mode simulations. Oh and Kim (2013) estimated the T-S law using a hybrid procedure, which combined both experimental measurements and inverse numerical computations. Blal et al. (2013) proposed a micro-mechanical-based criteria for the calibration of CCM parameters (cohesive peak stress, critical opening displacement, cohesive energy, etc.).

López et al. (2008a) developed a meso-scale fracture-based interface constitutive law, which is capable of simulating uniaxial tension/compression and biaxial
loading. Turon et al. (2010) imported an interlaminar strength and the penalty stiffness in CCM, to ensure correct energy dissipation when delamination propagates under mixed-mode loading. Park and Paulino (2012) implemented a new potential-based CCM in the FE package of ABAQUS, for mixed mode fracture simulations. Cuvilliez et al. (2012) coupled a gradient damage model and the CCM to simulated crack propagation in quasi-brittle materials under mode I loading condition. Evangelista Jr et al. (2013) introduced the 3D damage-based CCM with the thermodynamics of irreversible processes, which prevent previous cohesive states to change under external or local unloading.

Most of the newly developed CCMs are based on some specific FE codes or developed for specific problems, which are hard to utilise widely. The author thinks that the new forms (such as CCM mentioned in (Park and Paulino, 2011)) which are implementable or already exist in general-purpose FE packages are good choices. Besides, the development of methods of measuring the parameters, especially at micro-/ meso-scales, could strengthen the applications of CCM. Three-point bending and wedge-splitting tests (Peterson, 1980; Guinea et al., 1992), that are often used to determine the fracture energy at macro-scale, could be potentially used for micro-/ meso-scales. Luković et al. (2015) developed an experimental procedure for micro-mechanical testing (i.e. nano-indentation) of cement paste. The obtained micro-mechanical properties were directly used as input for numerical simulation of fracture behaviour of cement paste.

2.5.3 Cohesive element in ABAQUS

As mentioned above, various CCMs have been developed and reported in literature. In this research, the zero thickness cohesive element of CCM is used, which is available in the general-purpose FE package ABAQUS. There are three types of application in ABAQUS (ABAQUS, 2010), namely continuum-based modelling for a glue-like material which has a finite thickness, modelling of gaskets and/or laterally unconstrained adhesive patches, and traction-separation-based modelling for zero thickness interfaces. Thus, the zero thickness cohesive elements are initially inserted into the mesh. The detailed insertion procedure is introduced later.
Traction-Separation laws

The T-S law of CCM in ABAQUS, assumes that there exists tractions in the normal direction \((t_n)\) and two tangential or shear directions \((t_s\) and \(t_t)\) across the crack surfaces, caused by mechanisms such as material bonding, aggregate interlocking and surface friction in the fracture process zone.

A simple T-S curve \((t_n - \delta_n)\) with a linear softening law is illustrated in Figure 2-5. Before the crack initiates, a linear elastic ascending phase (OA) is assumed to describe the initial material without cracks. After the crack has initiated (A), the traction decreases monotonically as a function of the corresponding separation (AB), which is often termed tension or strain softening. Finally, the traction diminishes at the critical displacement (B). The unloading paths are also indicated. The areas under the curves (OAB) represent the mode-I fracture energy \(G_F\), which is treated as material properties. The initial tensile stiffness \(k_{n0}\) and the initial shear stiffness \(k_{s0}\) and \(k_{t0}\) should be high enough to represent the un-cracked material, but not too high to cause numerical ill-conditioning. These initial stiffness values can be determined by a trial and error approach. If \(\delta_n\) is negative during loading increments or iterations, a compressive stiffness of magnitude \(k_{n0}\) is assigned to prevent penetration of crack surfaces.

Figure 2-5 T-S curve with linear softening laws (Yang et al., 2009)
Computation of parameters

The CIE (e.g. COH2D4 in 2D or COH3D6 and COH3D8 in 3D) with zero in-plane thickness in ABAQUS, is based on the above cohesive crack model. The feature of CIE is that its formulation is based on the damage mechanics framework, within which the stiffness \( k_n \), \( k_s \) and \( k_t \) upon unloading and reloading are degraded as \( \delta_n \), \( \delta_s \) and \( \delta_t \) increase, due to irreversibly progressive damage. The damage is characterised by a scalar index \( D \), representing the overall damage of the crack caused by all physical mechanisms. It is a function of the so-called effective relative displacements \( \delta_m \) combining the effects of \( \delta_n \), \( \delta_s \) and \( \delta_t \):

\[
\delta_m = \sqrt{\langle \delta_n \rangle^2 + \delta_s^2 + \delta_t^2} \tag{2-2}
\]

where \( \langle \rangle \) is the Macaulay bracket and

\[
\langle \delta_n \rangle = \begin{cases} \delta_n, & \delta_n \geq 0 \text{ (tension)} \\ 0, & \delta_n < 0 \text{ (compression)} \end{cases} \tag{2-3}
\]

For the linear softening law in Figure 2-5, the damage can be calculated by

\[
D = \frac{\delta_{m,\text{max}}(\delta_{m,\text{max}} - \delta_{m0})}{\delta_{m,\text{max}}(\delta_{mf} - \delta_{m0})} \tag{2-4}
\]

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. An exponential softening law is also available in ABAQUS. The damage index \( D \) (known as variable SDEG) monotonically evolves from 0 to 1 upon further loading after the initiation of damage. Through Figure 2-5, once \( D \) is known, the stiffness \( k_n \), \( k_s \) and \( k_t \) can be calculated as:

\[
k_n = (1 - D)k_{n0} \tag{2-5}
\]

\[
k_s = (1 - D)k_{s0} \tag{2-6}
\]

\[
k_t = (1 - D)k_{t0} \tag{2-7}
\]

The tractions are affected by the damage according to
where $\bar{t}_n$, $\bar{t}_s$ and $\bar{t}_t$ are the traction components predicted by the elastic traction-separation behaviour for the current separation without damage.

Apart from the damage evolution law given by Equation (2-4), a damage initiation law referring to the beginning of stiffness degradation is also needed. ABAQUS contains several damage initiation laws. This study assumes a quadratic nominal stress law, i.e., the damage is assumed to initiate when a quadratic interaction function involving the nominal stress ratios reaches a value of one:

$$\left(\frac{<t_n>}{t_n^0}\right)^2 + \left(\frac{<t_s>}{t_s^0}\right)^2 + \left(\frac{<t_t>}{t_t^0}\right)^2 = 1$$  (2-11)

where $t_n^0$ and $t_s^0 = t_t^0$ represent the tensile strength and shear strength of the material, respectively.

For mixed-mode fracture energy criteria based on Benzeggagh-Kenane (BK) law (Benzeggagh and Kenane, 1996), is expressed as a function of the Mode I and Mode II fracture toughnesses:

$$G_F^c = G_{F_n}^c + (G_{F_n}^c - G_{F_s}^c)\left(\frac{G_s}{G_n + G_s}\right)^m$$  (2-12)

where $G_F^c$ is the total mixed-mode fracture energy;

$G_n$ is the normal strain energy release rate;

$G_s$ is the shear strain energy release rate;

$G_{F_n}^c$ is the normal fracture energy;

$G_{F_s}^c$ is the shear fracture energy;
Chapter 2 Literature Review

**Estimating the stable time increment**

In the ABAQUS/Explicit solver, the stable time increment for a cohesive element is equal to the time ($\Delta t$), which is required for a stress wave to travel across the constitutive thickness ($T_c$) of the cohesive layer:

$$\Delta t = \frac{T_c}{c} \quad (2-13)$$

where $c$ is the wave speed, and $E$ and $\rho$ represent the bulk stiffness and the density, respectively.

$$c = \frac{E}{\sqrt{\rho}} \quad (2-14)$$

So the stable time increment can be written as

$$\Delta t = T_c \sqrt{\frac{\rho}{E}} \quad (2-15)$$

For cases in which the constitutive response is defined in terms of traction versus separation, the slope of the curve is

$$k_n = \frac{E}{T_c} \quad (2-16)$$

And the density is specified as mass per unit area rather than per unit volume

$$\bar{\rho} = \rho \ T_c \quad (2-17)$$

Therefore, for the T-S law, the expression for the time increment becomes

$$\Delta t = \sqrt{\frac{\bar{\rho}}{k_n}} \quad (2-18)$$

It is quite common that the time increment for cohesive elements will be significantly less than that for the other elements in the model, unless actions are taken to alter one or more of the factors influencing the time increment. For simulations with ABAQUS/Explicit solver, the stable time increment could be used for estimation of the whole step time, as a longer one means greater stability.
but with a huge computational cost, while a shorter one will cause system instability.

2.6 Summary

Extensive research has been conducted, both on the multi-scale modelling methods and numerical characterisation of material heterogeneity. Either from a micro-mechanism or a multi-scale modelling point of view, it is clear that the micro information is crucially important and directly relates to localised behaviour, especially for fracture analysis where phenomena at the local nano- and micro-scales have a significant impact on the failure of structures at the meso- and macro-scales. However, most of the numerical models available in literature use assumed micro-/meso-scale morphologies, or assumed random field properties, rather than using direct and accurate representations of the internal structure of the materials. Therefore, the simulated damage and fracture processes cannot be directly and accurately validated.

In terms of non-destructive characterisation techniques, the ultrasound method has the advantage of being safe, fast, and cost-effective, but it is normally used for defect examination. Magnetic resonance imaging is widely used in medical and food science, however, it is rather expensive and reinforcement in a material (e.g. steel bars in concrete) sometimes causes problems. In comparison, X-ray computed tomography earned its primary position in material science by its high resolution, non-destructive nature, clear visualisation in 3D, and more importantly by its application in in-situ tests. Thus within this research, by combining the XCT and the state-of-the-art IBM technique, the realistic micro-structures of concrete is firstly characterised and then transformed into FE meshes for various simulations.

There are many numerical models for modelling crack propagation in quasi-brittle materials, such as the discrete crack model and the smeared crack model. They each have their advantages and disadvantages. The cohesive crack model appears to be extensively used, due to its capability of realistically representing
energy dissipation during the fracture processes, and the ease of its implementation as CIEs in FE Modelling.

As a typical engineering material, concrete has been widely used in many civil and industrial applications. Due to the random distribution of its multiple phases, the intrinsically heterogeneous mechanical properties at small-length scales directly determine the performance of structures at large scales. Therefore, the meso-scale in-situ characterisation and FE simulation has become an important and challenging task for both engineering application and scientific research.
This chapter presents the principles and detailed tomography results of in-situ X-ray computed tomography (XCT) experiments. The XCT characterisation technique is introduced. Then a Brazilian-like in-situ XCT test on a 40mm cube is presented as a benchmark work. Through detailed explanations of reconstruction and segmentation procedures, the segmented image model of the concrete specimen is shown, both without load and under maximum load. Two 20mm cubes were cropped and in-situ scanned under uniaxial compression and cyclic compression. Their fracture features were characterised and visualised through 2D tomography images and 3D volumes. The crack propagation, as well as the voids and cracks’ distribution, was characterised in 3D, throughout the load steps. The detailed distributions of aggregates and voids in deterministic concrete specimens were presented, which can be used for generating random concrete models. The segmented 3D imaging models were used for later image based FE simulations.

3.1 X-ray computed tomography

XCT is a technology that uses X-rays to produce tomographic images of a scanned object (or specific areas), allowing the user to see inside the specimen without cutting. Now it is widely used for medical imaging, as well as in many other fields, such as non-destructive characterisation of materials. The following sections briefly explain the procedures of a standard XCT experiment.
3.1.1 XCT process

Basically, XCT is based on the fact that different components of an object have different attenuation rates on an X-ray beam. Thereby, two-dimensional tomography layers can be stacked to generate three-dimensional images, where a virtual replica of the object is created to reveal its internal structure.

Similar to other computed tomography based imaging systems, XCT follows a basic set up. A sample is placed between an X-ray source and a detector. Then the sample is rotated while the X-rays hit the sample. After passing through the sample, the X-rays are detected. Finally, sequential images (slices) are collected and compiled to create 3D representations that can be manipulated digitally to perform measurement and visualisation tasks. Optimal data acquisition and interpretation require the proper selection of scanning configuration, use of suitable X-ray sources and detectors, careful calibration, selection of energy use, exposure and total scanning time, and special attention to origins and modes of artefact suppression (Ketcham and Carlson, 2001).

The quality of scanned images relies on many factors. The first one is the material type, as the amount of material attenuation of X-rays is controlled by the density and atomic number of each component. The second factor is the X-ray intensity, which controls its ability to penetrate the sample and affects the relationship between signal and noise in the image. High energy X-rays penetrate more efficiently than low energy X-rays. Therefore high energy X-rays can pass through a greater thickness of material or a similar thickness of denser material before they are absorbed. The energy of the X-ray beam should therefore be chosen carefully depending on the size and composition of the sample being investigated. On occasions, to obtain better contrast images, filters (e.g. copper or aluminium etc.) can be used before the X-rays reach the sample. The third factor is the distances between the X-ray source and the sample, and between the sample and the detector. Ideally, a closer distance between the sample and the X-ray source ensures better scanned quality. However, the X-rays should be emitted simultaneously across the sample’s width and should all be collected by the
detector. Finally, in order to obtain reliable slice images, the sample is fixed on the rotatable stage to ensure that it does not move while the X-ray is scanning.

3.1.2 Image reconstruction
The projection images that the detector collects are stored and need to be reconstructed. This mathematical process is called image reconstruction, which converts projection images into 2D grey level slice images. The most widespread reconstruction technique is called filtered back-projection, in which the data are first convolved with a filter, to create a set of filtered views. Each view is successively superimposed over a square grid at an angle corresponding to its acquisition angle. After reconstruction, the raw projection data are converted to CT numbers, or grey values, that have a certain range determined by the computer system (e.g. 8-bit/ 16-bit etc.).

Tomography combines the information of many projection images, each taken at a different orientation and is related to the movement of the X-ray rotation stage. The stage is the base that seats the sample, which can be adjusted to specific horizontal, vertical, magnification and tilt axes. Figure 3-1 illustrates the XCT acquisition and reconstruction processes. Whilst scanning, it rotates the sample by 360 degrees (or 180 for certain conditions). Rotating the stage at a slower rate increases the number of projections taken, thus enhancing the reconstruction and prolonging the total scanning time. When the angular step between each projection is small, it is possible to compute the attenuation coefficient at each point of the sample. Projections taken at different orientations are combined to output an image reconstruction. The reconstructed image is in the form of pixels in 2D (unit of picture in 2D) or voxels in 3D. Each pixel, or voxel, in the reconstruction is allocated a grey value, from a grey scale, as a representation of the attenuation coefficient of the element occupying that pixel/voxel.
3.2 Brazilian-like in-situ XCT test

As it is non-destructive, XCT has been used in many disciplines to capture the internal features of composites, and the in-situ XCT characterisation of damage and fracture under progressive load has received more and more attentions. Recently, a benchmark Brazilian-like in-situ XCT test of a 40mm concrete cube was conducted (Yang et al., 2013), which allows 3D visualisation and characterisation of damage propagation during continuous loading.

3.2.1 Experiment

The in-situ XCT experiments of concrete cube specimens under Brazilian-like compression were carried out, as a benchmark work of this research, at the Manchester X-ray imaging facility, at the University of Manchester, UK. The used 225/320 kV Nikon Metris custom bay and the DEBEN loading system are shown in Figure 3-2a. Figure 3-2b shows the concrete specimen at failure, in which the loading area of 17.5×17.5 mm² is highlighted (i.e. 19% of the sample cross-sectional area).
The DEBEN system (screw-driven loading) (Mostafavi et al., 2013b) was used to apply compressive load to the specimen, which was positioned on a rotating stage. The Perspex tube allows live observations, both by projection and sight view. The different X-ray attenuation of concrete ensures no significant effects come from the tube or outside the specimen. Many combinations of the exposure time, voltage and beam current were tried and the best one was selected in terms of the best resultant image quality and the reasonable scanning time. Finally, the X-ray projections were acquired with an exposure time of 2s at an accelerating voltage of 160kV and a 60μA beam current using a tungsten target. For each scan, the stage was rotated through 360 degree, resulting in 2000 projections collected on a Perkin Elmer 2048×2048 pixel amorphous silicon flat panel detector with an effective pixel size of 37.2μm.

The concrete cube specimens, of 40 mm size with a target compressive strength of 15 MPa, were cast in the laboratory. This target strength and size of the specimens were chosen so that the specimens could be loaded to failure using a 25kN loading rig that could be accommodated within the XCT instrument. The ordinary Portland cement and gravel aggregates with an average size 5 mm, were used. No fine aggregates (i.e. sand) were used, to ensure a relatively simple internal structure for analysis.
Figure 3-3a illustrates the loading curve of the in-situ XCT test procedure. The displacement control loading scheme was used in order to ensure there would be no further movement during each scan, which otherwise would generate blurred images. The first scan was conducted without loading. The load was then applied via compression (in $z$ direction) at a displacement rate of 0.5mm/min to 2.5kN, at which point the second scan was carried out. After the load was released, the specimen was reloaded to 6kN at the same rate and the third scan was undertaken. The fourth scan was conducted at 10kN and the fifth at 16.5kN, after which macro-cracks appeared in a side surface and widened quickly. For each scan, the standard X-ray scanning procedure was utilised (Onifade et al., 2013), which includes the specimen set-up, machine warming up, pre-scan settings, energy checking, exposure time selection, detector and CT calibration etc. The displacement load was maintained during each scan. The 16.5kN was considered as the peak load during the experiment. Furthermore, a post scan was conducted at a same loading rate up to 13.5kN, at which point the specimen was totally damaged.

Figure 3-3 The loading curve of the benchmark in-situ XCT test (Yang et al., 2013)

3.2.2 Reconstruction
A 3D attenuation contrast image was computationally reconstructed using a filtered back projection algorithm, using the projections comprising each dataset.
CT Pro, VG Studio and AVIZO software packages were used to reconstruct, visualise and segment the raw datasets, which consist of 2000 slices and require 15 GB storage. The 3D images were rotated and cropped to align every dataset. To reduce the data processing time and possible edge effects, a 37.2mm cube region of interest was cropped from the 40 mm cube volume. After reconstruction, the 3D data size was reduced to 2 GB for each scan. The bit depth was reduced from 32 bit to 16. It contains 1000 slices in each direction with a resolution of 37.2μm. Figure 3-4 shows the workflow of the reconstruction process.

![Workflow of reconstruction process]

As a benchmark test, the samples were cubes. From the reconstructed data in Figure 3-4, a clear difference of the grey value was found for the same phase (such as cement) for places at boundaries and in the centre. This is caused by the well-known beam hardening effect (Landis et al., 2003), which was reduced using filters in AVIZO, such as background and flat field correction. In addition, it is worth noting that beam hardening can also be eliminated by adjusting the X-ray beam energy, or using both the source and back filters, when collaborating the XCT scan.

Figure 3-4 Workflow of reconstruction process
Chapter 3 In-Situ X-Ray Computed Tomography Experiment

3.2.3 Digital volume correlation
As the DEBEN system recorded a soft force-displacement curve in Figure 3-3, the reconstructed image datasets were used to perform digital volume correlation (DVC) analysis, using the LaVision Davis software (DaVis, 2012). DVC, coupled with 3D imaging techniques such as XCT, enables the measurement of full 3D displacement and strain fields interior of a material. It provides an experimental compliment to validate the 3D FE simulations (Gates et al., 2011; Yang et al., 2013) and can also play a vital role in determining input parameters for simulations (Gates et al., 2015).

DVC starts with processing a random internal pattern of features in a sample, that detected by 3D imaging techniques. This internal “speckle” pattern can arise either from inherent micro-structure or by embedding particles on purpose (Gates et al., 2011; McDonald and Withers, 2014). By 3D imaging techniques, a reference image of the un-deformed sample is first captured. Then, after some deformation is applied, an image of deformed sample is characterised either in-situ or ex-situ. For a specified 3D volume, DVC determines the deformation that maps the volume in the reference image to the volume in the deformed image with the best correlation. This mapping is given by a shape function. In general, the two volumes do not exactly match, however the best possible match can be found by optimizing the objective function.

In DaVis, the displacement field was analysed using progressively smaller volume subsets (i.e. interrogation windows) to obtain the relative positions and deformation (Mostafavi et al., 2013b; McDonald and Withers, 2014; Mostafavi et al., 2014; Mostafavi et al., 2015). The rigid body movements and rotations between datasets were corrected by visual matching of image slices, so that the displacement field coordinate system was aligned. The 6kN scan was ignored due to the blurred XCT images. The parameters used in the DVC calculation were: interrogation window size of 128×128×128 voxels, 50% overlap and 2 passes. Reducing the final interrogation window size increases the spatial resolution of the displacement field. In the meantime, the random errors also increase (Mostafavi et al., 2015). The displacement at each load step was
calculated by subtracting the top and bottom slices that were perpendicular to the load direction.

The modified force-displacement curve, with displacement error bars, is shown in Figure 3-5. Although a large deviation was involved, a more realistic estimation of the elastic modulus of the concrete cube was calculated as 20GPa, by conducting liner fit up to 10kN (see red line in Figure 3-5). This modified curve was used for later 3D validation of FE simulation.

![Figure 3-5 Modified force-displacement curve by DVC](image)

3.2.4 3D segmentation

Segmentation is the process of identifying different phases in a composite volume. The commercial software AVIZO (AVIZO, 2013) was used for segmentation in this study. It is a powerful, multi-faceted tool for visualising, manipulating, understanding 3D image datasets, and advanced qualitative and quantitative analysis. 3D surfaces of different phases in concrete can be reconstructed through the segmentation process. Figure 3-6 shows the AVIZO software interface. The 3D Viewer shows visualisation results obtained with the different modules that are used. The project pool contains icons representing data and modules. The module’s input and parameters are displayed in the properties area.
In AVIZO, voxels of different material are labelled either manually or automatically, and added or subtracted to a particular material set. The dataset under 16.5kN is taken as an example to illustrate the segmentation procedure. The detailed workflow is presented in the following sections.

**Data import**

The reconstructed raw datasets were imported into AVIZO with the dimensions of 1000×1000×1000 voxels and the voxel size of 37.2μm. Figure 3-7 shows the imported slice views, showing the phases of concrete: aggregate, cement, voids and cracks.
Image quality improvement

Prior to segmentation, the MEDIANFILTER3D and UNSHARP-MASK filters were used to improve the image quality and reduce noises. The MEDIANFILTER3D (AVIZO, 2013) command uses morphological operators to set the pixel value to the median for the defined neighbourhood. The grey levels of all pixels in the neighbourhood are sorted, from the smallest to the largest value. The median value is then calculated. The process may be iterated. The UNSHARP-MASK filter (AVIZO, 2013) sharpens edges of the elements without increasing noise. It first applies a Gaussian filter to a copy of the original image and blends it with the original. Undesired effects are finally reduced by using a mask to only apply sharpening to desired regions. Figure 3-8 shows the image before and after applying the filters.

Line probe study

The next step is to identify the proper value of the thresholds for segmentation. Since the phases of aggregate, cement and voids have different densities, the different attenuation of the X-rays will lead to different grey values. Thus the most straightforward way for segmentation is using threshold values to distinguish the phases. According to the density values, the aggregates had the highest intensity, followed by cement and voids.
In AVIZO, the LINE-PROBE command was used to inspect the scalar data in the fields. The probes are taken along a line from one point to another within the sample. The grey values vary along this line, see line AB in Figure 3-9a. The 16-bit image contains grey level in a range of 0 to 65535. The average value for each phase can be estimated. Two critical dividing lines were drawn, which were on the values of 19000 and 33000. However, the micro-void in the left part of the Figure 3-9a was divided into the cement phase, which is not right. Here the comprise was made that small voids, especially with small volume in 3D, were not considered in the segmentation process. Therefore, they were ignored for later 3D FE simulations as well.

![Line-probe path](image1)

(a) Line-probe path

![Grey values along the probe line AB](image2)

(b) Grey values along the probe line AB

Figure 3-9 Line-Probe grey values across a xy plane slice
Grey-scale-based segmentation

Then, the LABEL-FIELD function in AVIZO was used to create new label files, where the corresponding threshold values were assigned to different phases. According to the line probe study, the threshold value for voids was 0 (minimum)-19000, 19000-33000 for cement, and 33000-65535(maximum) for aggregates. As shown in Figure 3-10, the segmentation result of a central $xy$ slice was not ideal. The central part looked clear, but the boundary regions are blurred. Some of the aggregates were connected and some had holes inside.

Further operations such as growing, shrinking and smoothing were conducted to improve the segmented images. The BRUSH and BLOW commands were used to disconnect aggregates and eliminate the areas smaller than several (15 in this study) pixels for all slices. In order to reduce the amount of these tedious operations, the original 1000 slices with a resolution of 37.2$\mu$m were re-sampled to a 372 slices cube with a resolution of 0.1mm before manual interactions. The re-sample operation in AVIZO shrinks the dimension of the image data from the original resolution to a new one, in which interpolations may involve.

The segmentation of the aggregate phase was completed first (see Figure 3-11a). This was followed by the voids (including cracks in the dataset of 16.5kN, see Figure 3-11b). The cement phase was then obtained by subtracting the aggregates and voids from the whole image (see Figure 3-11c).
Chapter 3 In-Situ X-Ray Computed Tomography Experiment

Figure 3-11 The segmented binary images: (a) aggregate, (b) voids and (c) cement, black areas represent background.

All the segmented phases were then combined together into a whole “digital” concrete cube using ARITHMETIC, as visualised in Figure 3-12a. The separate phases are shown in Figure 3-12b-d. The major cracks on the specimen surface in Figure 3-12a and d are roughly vertical, which is a feature of concrete specimens fractured under compression.

Figure 3-12 The 3D views of concrete cube under 16.5kN (loading was under \( z \))
The 3D image dataset of the sample at zero loading was also segmented following the same procedure above. The 3D visualisation is shown in Figure 3-13a-d. Comparison of Figure 3-12d and Figure 3-13d clearly demonstrates the effects of loading on the crack propagation. The complex multi-crack pattern is essentially 3D. Although both the specimen geometry and the loading and boundary conditions are almost symmetric, the crack pattern is not symmetric. This reflects the effects of the random distribution of aggregates and thus the heterogeneous nature of mechanical properties of concrete. The segmented phases in Figure 3-13 were used for later 2D and 3D FE simulations. Theoretically, multiple specimens need to be repeated to ensure the results are statistically representative. However, here as a trial test, only one specimen was tested to build the frame work of this study. The specimen size of 40mm was selected due to the capacity of the DEBEN loading system.

![Figure 3-13 The 3D views of concrete cube without load](image)
The volume fraction of each phase in the segmented 40mm cube without load is shown in Table 3-1. The aggregate and cement have close volume fractions of 49.6% and 49.7%, respectively, while 0.7% volume are the voids.

<table>
<thead>
<tr>
<th>Volume (mm³)</th>
<th>Fraction (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aggregate</td>
<td>25533.3</td>
</tr>
<tr>
<td>Cement</td>
<td>25571.8</td>
</tr>
<tr>
<td>Voids</td>
<td>373.9</td>
</tr>
<tr>
<td>Total</td>
<td>51479</td>
</tr>
</tbody>
</table>

3.2.5 Evolution of voids and cracks

The volume fraction of the voids and cracks (with grey values lower than 19000) in the specimen under different loads were calculated. Figure 3-14 shows the volume fractions at various loads. The observed volume of voids and cracks first decreases as the load increases. This is attributed to compaction of the concrete under compression. This causes part of the observed void population to fall below the detection threshold of the XCT at this resolution. As the load increases further, cracks gradually occur, leading to a higher volume of cracks and voids. Near and after the peak load, major vertical cracks propagate fast, leading to dilation in the specimen.

Figure 3-14 Volume evolution of voids and cracks
3.3 Uniaxial compression in-situ XCT test

3.3.1 Experiment
A uniaxial compression in-situ XCT test of a 20mm concrete cube (marked as number 2), cut from the same batch of concrete as the 40mm cube, was conducted using the same XCT facility and the DEBEN loading system as in Figure 3-2a. The difference is that the loading and constraint areas were top and bottom surfaces (in z-direction). As the sample size was halved, different X-ray scanning parameters were applied to ensure a faster and more accurate scan: the exposure time was 1.4s; the accelerating voltage was 100kV and the beam current was 200μA. A total of 1500 projections with 16.5μm pixel size were obtained. Other settings were maintained. Figure 3-15 shows the sample before loading. A missing corner can be seen, which was caused by cutting operation. The same standard XCT procedure used in the Brazilian-like test was performed. The artificial defects such as beam hardening and ring effects reduce the quality of scanned images and hence affect later segmentation results. They were minimised and further corrected by post-processing using CT Pro (e.g. finding the true centre of rotation) and AVIZO (e.g. using background and flat field correction filters).

Figure 3-15 The in-situ sample before applying load
Chapter 3 In-Situ X-Ray Computed Tomography Experiment

The loading history is shown in Figure 3-16. The initial scan labelled as 0kN was taken without any load. Compressive loading was then applied at a displacement rate of 0.05 mm/min in z-direction up to 0.8kN, at which point the second scan was conducted. Then the load was increased to 2kN at the same rate and a third scan was undertaken. Similarly, the fourth, fifth and sixth scans were conducted at 3kN, 5kN and 9.1kN, respectively. It took around half an hour for each scan. During each scan, the load was set to be maintained; however, the recorded load value showed a small reduction (around 0.1kN). The load was slightly relaxed when the loading motor was stopped. Similar image reconstruction process like Brazilian-like test was conducted. The 8 bit image with grey values ranging from 0 to 255 was outputted for later image processing.

From Figure 3-16, similar to the 40mm cube test, a soft force-elongation curve was obtained, mainly due to the compliance from DEBEN system. Thus, the 3D displacement field within the sample along the whole loading history were recalculated by DVC. The rigid body movements and rotations between datasets were corrected. The parameters used in the DVC calculation were: window size of 128×128×128 voxels, 50% overlap and 2 passes. The displacement at each load step was calculated by subtracting the top and bottom slices that were perpendicular to the loading direction. Figure 3-17 shows the modified force-displacement curve for sample 2 under uniaxial compression. The linear fit (red line in Figure 3-17) from 0N up to 3kN gives an elastic modulus of 23.6GPa. This curve is different from the Brazilian-like 40mm test in Figure 3-5. The

![Figure 3-16 The loading history for sample 2](image-url)
primary reason may because of different loading schemes. Uniaxial compression of sample 2 was loaded on the whole top and bottom surfaces, while the Brazilian-like test was loaded and constraint on concentrated areas (19% of the surfaces). The different sample sizes and sample variations may also play important roles. This curve was used for later validation of the 3D image based FE simulation.

![Figure 3-17 The modified F-d curve of sample 2 by DVC](image)

### 3.3.2 The damaged sample

The damaged sample after the final scan is shown in Figure 3-18. Several surface cracks were seen after unloading, and one corner of the sample actually dropped off when the sample was removed. The target compressive strength was 15MPa, and the peak load of the 40mm concrete cube under the Brazilian-like loading was 16.5kN (see the section above). Thus the estimated peak load of this 20mm cube is 6kN. However, the sample had not disintegrated at 9.1kN and could have sustained more loading. This may be because the majority of the load was carried by strong aggregates, as the sample size 20mm is only 4 times the average aggregate size (5mm). The detailed internal damage can be visualised from scanned CT images and segmented visualisations, which will be introduced in the following sections.
3.3.3 Fracture observed from 2D tomography slices

Figure 3-19 illustrates micro-cracking using vertical tomography images (slice in $xz$ direction, which is parallel to the loading direction.) at different loading stages. The $xz$ slices may not be the precise ones under each load, however the best matches were tried and the qualitative results were concluded. For the loads less than 3kN, there were few differences in terms of micro-crack patterns. However, gradual volume expansion in the horizontal direction ($X$) was found throughout, due to the compression of the bottom rig. As the load increased from 3kN to 5kN, a vertical contraction occurred and multiple cracks were generated, including new cracks near the cube surface, propagation of micro-cracks and even cracks in the aggregate. For loads under the maximum value (9.1kN), multiple cracks propagated continuously and crack diversion occurred when the cracks reached the aggregate.
3.3.4 Sub-volume micro-cracking

A small sub-volume was cropped from the damaged region of the sample. Figure 3-20 illustrates the localised cracking and damage propagation. The almost same position in the sample was selected for different loading conditions. Again, few differences were noticed before 3kN. From 3kN to 5kN, multiple micro-cracks appeared, mainly in the cement and on the aggregate-cement interfaces. Crack opening and closing was visualised by comparing Figure 3-20a, b and c. Meanwhile, crack bridging was clearly characterised between nearby interfacial cracks. Under 9.1kN, the main damage occurred and multiple cracks were found even in aggregates.
Furthermore, the cracks were segmented for the sub-volumes under 5kN and 9.1kN. Figure 3-21 and Figure 3-22 show the 3D crack surfaces and the cracking of three slices. The propagation of 3D crack surfaces illustrates realistic damage evolution within the sample. From the slice views at the same location, the aforementioned cracking features such as opening, propagation and bridging were also unveiled. It is clear that the cracks first propagated along interfaces between aggregate and cement or between aggregates (aggregate 1 and 2 in Figure 3-21). Then either bridging or diversion occurred when they were propagating.
Figure 3-22 3D crack surface and slice views at the same location as Figure 3-21

3.3.5 3D segmentation

Phase segmentation

For the ease of segmentation, the 3D image cube was cropped to a 195×191×207 mm$^3$ volume (i.e. 7710 mm$^3$), and the image resolution was reduced to 0.1mm. The same procedure as in Section 3.2.4 for the 40mm cube was applied to segment the phases in this volume. The 3D segmentation results at 0kN load are shown in Figure 3-23. The different colours in Figure 3-23a represent different aggregates. The cement paste is like a porous volume. The initial defects (the missing corner and initial pores) are visualized in the voids phase.
The volume fraction of each phase in the segmented cube is shown in Table 3-2. When exclude the missing corner, the total volume is 7673 mm³. The aggregate occupies the most volume at 55.0%, followed by the cement paste at 44.3%. The total defects excluding the missing corner have a value of 0.7%.

<table>
<thead>
<tr>
<th></th>
<th>Volume (mm³)</th>
<th>Fraction (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aggregate</td>
<td>4222</td>
<td>55.0</td>
</tr>
<tr>
<td>Cement</td>
<td>3402</td>
<td>44.3</td>
</tr>
<tr>
<td>Voids</td>
<td>49</td>
<td>0.7</td>
</tr>
<tr>
<td>Total</td>
<td>7673</td>
<td>100</td>
</tr>
</tbody>
</table>

**Aggregate size distribution**

Figure 3-24 shows the distribution of aggregates in terms of the volume. There are 108 aggregates in total. From Figure 3-24, it can be concluded that the volume of most aggregates is in the range of 1-20 and 30-60 mm³. Table 3-3 shows the statistical analysis of the results. The mean volume, length and width are 39.09 mm³, 7.37 mm and 2.74 mm, respectively. The mean equivalent diameter is 3.88 mm, with a standard deviation of 1.24 mm.
Figure 3-24 3D volume distribution for aggregates in sample 2

Table 3-3 Statistical analysis for aggregates in sample 2

<table>
<thead>
<tr>
<th></th>
<th>Volume (mm³)</th>
<th>Equivalent Diameter (mm)</th>
<th>Length (mm)</th>
<th>Width (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>39.09</td>
<td>3.88</td>
<td>7.37</td>
<td>2.74</td>
</tr>
<tr>
<td>Min</td>
<td>0.02</td>
<td>0.31</td>
<td>0.83</td>
<td>0.20</td>
</tr>
<tr>
<td>Max</td>
<td>112.11</td>
<td>5.98</td>
<td>12.25</td>
<td>5.91</td>
</tr>
<tr>
<td>Standard deviation</td>
<td>26.32</td>
<td>1.24</td>
<td>2.22</td>
<td>1.11</td>
</tr>
</tbody>
</table>

**Voids size distribution**

The missing corner with a volume of 37 mm³ was generated during preparation, thus was excluded for voids’ size distribution. There are 51 voids in total. Figure 3-25 shows the 3D volume distribution. Table 3-4 lists the statistical results. The mean volume is 0.88 mm³. It is obvious that for 84% (43 out of 51) of the voids, their volume is less than the average value. The maximum void has a size of 18.65 mm³. The mean equivalent diameter, 3D mean length and width are 0.72 mm, 1.67 mm and 0.63 mm respectively. The distribution information of calculated aggregates and voids can be used for generating random concrete structures (Yin et al., 2013; Wang et al., 2015b).
Chapter 3 In-Situ X-Ray Computed Tomography Experiment

Figure 3-25 3D volume distribution of voids in sample 2

Table 3-4 Statistical analysis for voids in sample 2

<table>
<thead>
<tr>
<th></th>
<th>Volume (mm$^3$)</th>
<th>Equivalent Diameter (mm)</th>
<th>Length (mm)</th>
<th>Width (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>0.88</td>
<td>0.72</td>
<td>1.67</td>
<td>0.63</td>
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<td>Min</td>
<td>0.001</td>
<td>0.12</td>
<td>0.11</td>
<td>0.11</td>
</tr>
<tr>
<td>Max</td>
<td>18.65</td>
<td>3.29</td>
<td>8.47</td>
<td>2.38</td>
</tr>
<tr>
<td>Standard deviation</td>
<td>2.80</td>
<td>0.62</td>
<td>1.79</td>
<td>0.57</td>
</tr>
</tbody>
</table>

3.3.6 Crack propagation in 3D

The segmentation of voids and cracks was relatively straight-forward in comparison with other phases in concrete (i.e. aggregate and cement), as they are usually empty dark areas in the tomography images. Thus, simple grey-scale based segmentation was used to segment the voids and cracks during the loading history. The XCT slice and segmented image at 9.1kN load are shown in Figure 3-26 a and b. It can be seen that most voids and cracks were captured. However, a large number of tiny micro-cracks were not identified, especially for those small volumes less than 15 pixels in 3D.
The 3D crack propagation during the loading history is presented in Figure 3-27, in which Figure 3-27a shows the initial defects of the sample at 0kN, including micro-cracks, uneven edges, inner pores and the missing corner. Figure 3-27b, c and d show the distribution of cracks for the load steps 3kN, 5kN and 9.1kN (compared with Figure 3-27a), respectively. Few differences were observed before 3kN. The volume of voids and cracks increased gradually towards 5kN, due to the propagation of micro-cracks (Figure 3-27c). At 9.1kN, a large number of new vertical (Z) cracks were noticed, mostly concentrated in the severely damaged corner in Figure 3-18.
3.3.7 Evolution of voids and cracks

Figure 3-28 shows the evolution of the volume fraction of voids and cracks during the loading. As the slices near the surfaces have very high volume fractions due to the uneven edges and the missing corner, only the middle 1213 slices (out of total 1243) along the height (Z) direction were used herein. The total volume of voids and cracks first decreases as the load increases (from 0kN to 3kN). This is attributed to compaction of the concrete under compressive load. As the compressive load increased further, cracks gradually propagated, leading to a higher total volume up to 5kN. At the peak load (9.1kN), major vertical cracks propagated (Figure 3-27d), and this caused the dilation of the whole sample. Compared with the crack volume change in the 40mm cube (Figure 3-14), a similar trend can be seen.
Figure 3-28 Volume evolution of voids and cracks

Figure 3-29 shows the area fractions of voids and cracks of the 1243 horizontal slices along the sample height direction (Z) for each load step. For every slice, the area fraction of voids and cracks was calculated and then plotted along the sample height. Figure 3-29 shows that there is inherent inhomogeneity in terms of voids and cracks both before and after loading. This inhomogeneity strongly influences the overall mechanical responses of the composites (Elseifi et al., 2011).

(a) at 0/0.8/2/3 kN     (b) at 3/5/9.1 kN

Figure 3-29 The voids and cracks contents along the height direction during loading

From Figure 3-29, it can be seen that the top and the bottom parts of the sample have 2% to 5% content of voids and cracks, and the middle 82% part has less...
than 2%. It has been reported that the larger air voids were normally concentrated at the top and bottom parts of concrete samples (Masad et al., 2002; You et al., 2009; Elseifi et al., 2011). In the present study, the reason for the large content of voids on top is due to the natural forming process, as multiple large pores exist in 3D (see top of Figure 3-27a). However, high porosity at the bottom comes from the corner defect: a large missing corner (see bottom of Figure 3-27a), which was caused during the sample preparation. The middle parts of the curves have a few peaks, representing one or more large pores (see the middle of Figure 3-27a). Such initial defects and heterogeneous micro-structures significantly intensify the transverse tensile strains during compression and stress concentration around the pores, and the voids provide weak regions where crack propagation is accelerated (Yuan and Harrison, 2005; Erdem et al., 2012).

Figure 3-29a shows that during loading the content of voids and cracks first decreased from 0N to 0.8kN. However, there were few differences for the loads of 0.8kN, 2kN and 3kN. Then the total volume of voids and cracks gradually increased (see Figure 3-28), especially in the regions near large pores (see the difference between the curves for 3kN and 5kN in Figure 3-29b). Finally the volume of voids and cracks reached its maximum value at 9.1kN.

3.3.8 Crack width and ITZ thickness measurement
The high resolution micro-XCT images are used in this section to measure important fracture properties, including the crack width and the thickness of interfacial transition zones (ITZ). They will not only provide inputs for numerical modelling, but also shed insights on fracture mechanisms, such as the length of fracture process zone etc.

Crack width
The distributions of grey values across cracks at three different locations shown in Figure 3-30 were analysed in a selected slice image (xz324 under 9.1kN). As an example, the average distribution of line 1 to 6 at location 1 is shown in Figure 3-31. The grey value was roughly constant until position A, and then started to decrease quickly to the valley B; after a flat stage to the other side of
valley (position C), it started to increase quickly until D and finally became constant again until its last position E. Three distinct regions were drawn as: OA, AD and DE, corresponding to cement (OA), crack (AD) and aggregate (DE), respectively in this example.

Figure 3-30 Crack locations

Figure 3-31 The average grey value distribution of line 1 to 6 in Figure 3-30

It’s clear that the flat valley is the crack centre, adjacent to a crack transition zone (CTZ) on each side. In order to minimise the measurement error, the maximum and minimum widths are considered as the distance between top branches (AD) and the distance of flat bottom of the valley (BC). The measured maximum and minimum widths for each line (18 in total) in Figure 3-30 are shown in Table 3-5. The CTZ width was calculated as half of the difference between average-maximum and average-minimum values (CTZ = (Max-Min)/2). From Figure 3-30 it is noticeable that the crack at location 1 (from 1 to 6) is the widest, followed by locations 2 and 3. Correspondingly, the results in Table 3-5 show that the CTZ width at location 1 has the largest value of 0.088mm, and that at location 3 has the smallest 0.052mm. The average crack width calculated as a mean of the maximum and minimum widths is 0.122, 0.094 and 0.084 mm for location 1, 2 and 3, respectively. AVG means average value.
## Table 3-5 Crack widths measured from Figure 3-30

<table>
<thead>
<tr>
<th>Location 1</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>AVG (mm)</th>
<th>CTZ (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>crack max</td>
<td>0.281</td>
<td>0.219</td>
<td>0.198</td>
<td>0.177</td>
<td>0.199</td>
<td>0.188</td>
<td>0.210</td>
<td>0.088</td>
</tr>
<tr>
<td>crack min</td>
<td>0.031</td>
<td>0.031</td>
<td>0.021</td>
<td>0.031</td>
<td>0.062</td>
<td>0.027</td>
<td>0.034</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Location 2</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
<th>11</th>
<th>12</th>
<th>AVG (mm)</th>
<th>CTZ (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>crack max</td>
<td>0.143</td>
<td>0.163</td>
<td>0.123</td>
<td>0.204</td>
<td>0.173</td>
<td>0.184</td>
<td>0.165</td>
<td>0.071</td>
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<tr>
<td>crack min</td>
<td>0.02</td>
<td>0.031</td>
<td>0.034</td>
<td>0.031</td>
<td>0.01</td>
<td>0.01</td>
<td>0.023</td>
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</table>

<table>
<thead>
<tr>
<th>Location 3</th>
<th>15</th>
<th>16</th>
<th>17</th>
<th>18</th>
<th>/</th>
<th>/</th>
<th>AVG (mm)</th>
<th>CTZ (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>crack max</td>
<td>0.119</td>
<td>0.155</td>
<td>0.137</td>
<td>0.131</td>
<td>/</td>
<td>/</td>
<td>0.135</td>
<td>0.052</td>
</tr>
<tr>
<td>crack min</td>
<td>0.037</td>
<td>0.037</td>
<td>0.027</td>
<td>0.026</td>
<td>/</td>
<td>/</td>
<td>0.032</td>
<td></td>
</tr>
</tbody>
</table>

* AVG means average.
The average curves of grey value distributions at three locations, with standard deviation, are shown in Figure 3-32. The AVG 1, 2 and 3 in the legend represent the average value at locations 1, 2 and 3 respectively. From this figure, suggestions can be made for grey-scale-based segmentation of this 20mm cube: grey values over 48 could be considered as aggregate, areas with grey values smaller than 45 as voids and cracks, and those in between 45 to 48 as cement.

![Average curves of grey value distributions for location 1, 2 and 3](image)

Figure 3-32 Average curves of grey value distributions for location 1, 2 and 3

**ITZ thickness**

The aggregate-cement ITZ thickness is an important material parameter for FE simulations based on continuum damage mechanics, but its accurate value is difficult to obtain by experiments due to the small size involved and thus often assumed. For example, (Xiao et al., 2013a; Xiao et al., 2013b) used nano-indentation to measure the ITZ thickness, but a smooth and flat surface need to be guaranteed by atomic force microscopy. Herein an effort was made to measure the thickness of the ITZ directly from XCT images. Similar to the measurements of crack width, the distribution of grey value unveils the transition from one phase to another when crossing boundaries of phases. Thus the thickness of the ITZ can be regarded as the distance between two phases when lines across the interfaces are drawn. Four locations investigated are shown in Figure 3-33. The average curve of all the 20 lines is shown in Figure 3-34.
As shown in Figure 3-33, the ITZ are considered as the area where there is a big change in terms of grey value, and the dividing points are selected at the positions where the gradient becomes relatively small. The measurements of the ITZ thickness are shown in Table 3-6. The final mean and the standard deviation for the 20 locations are 0.157mm and 0.028mm. To obtain a statistical value, multiple specimens are needed.
## Table 3-6 The measurement of the ITZ thickness at different locations

<table>
<thead>
<tr>
<th>Location</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
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<th>9</th>
<th>10</th>
<th>11</th>
</tr>
</thead>
<tbody>
<tr>
<td>ITZ</td>
<td>0.180</td>
<td>0.154</td>
<td>0.167</td>
<td>0.192</td>
<td>0.178</td>
<td>0.187</td>
<td>0.155</td>
<td>0.189</td>
<td>0.155</td>
<td>0.193</td>
<td>0.147</td>
</tr>
<tr>
<td>Location</td>
<td>12</td>
<td>13</td>
<td>14</td>
<td>15</td>
<td>16</td>
<td>17</td>
<td>18</td>
<td>19</td>
<td>20</td>
<td>AVG</td>
<td>SD</td>
</tr>
<tr>
<td>ITZ</td>
<td>0.136</td>
<td>0.129</td>
<td>0.096</td>
<td>0.099</td>
<td>0.134</td>
<td>0.166</td>
<td>0.177</td>
<td>0.154</td>
<td>0.159</td>
<td>0.157</td>
<td>0.028</td>
</tr>
</tbody>
</table>

* AVG means average; SD means standard deviation.
3.4  Cyclic compression in-situ XCT test

3.4.1  Experiment

Another 20mm cubic sample (marked as number 4) was tested under cyclic compressive loading on the same in-situ XCT facility (Figure 3-2a). The X-ray scanning parameters were: exposure time of 1.4s, accelerating voltage of 100kV and beam current of 200μA. The resultant data were 1500 projections with a 16.6μm pixel size.

Figure 3-35 shows the sample before the test. The loading history is shown in Figure 3-36. There were three cycles of loading and unloading. The initial scan (A) was taken without any load, which was labelled as 0kN. After that, the load was applied at a displacement rate of 0.5 mm/min to 7kN. With the displacement in place, the second scan (B) was conducted. Then the force was unloaded to nearly 0 (0.06kN), and the third scan (C) was carried out to complete the first load cycle. Similarly, the second load cycle with the fourth (D) and fifth scans (E), and then the third load cycle with the sixth (F) and seventh (G) scans were performed, with maximum loads of 10kN and 24kN, respectively. It took around half an hour for each scan.

![Figure 3-35 Sample 4 before test](image1)

![Figure 3-36 The loading history of sample 4](image2)

3.4.2  Characterisation of fracture features

The damaged sample after the final scan is shown in Figure 3-37, where some of the surface cracks are visible. The detailed characterisation of the fracture
features was carried out from two perspectives: the overall damage of the whole sample and the localised behaviour in sub-volumes. These are illustrated in detail in the following sections.

![After load](image.png)

Figure 3-37 The damaged sample 4 under cyclic compression

**Overall damage of the whole sample**

The overall damage process was illustrated through observations of the 2D tomography slices (slice in \(xz\) direction) at different load stages, see Figure 3-38. The 2D slices were extracted from scanned 3D image data at roughly the same location. The load stages, at positions of A, B, D and F in Figure 3-36, were used to demonstrate the damage propagation caused by the loading process.
Chapter 3 In-Situ X-Ray Computed Tomography Experiment

Figure 3-38 Fracture observed from 2D slices (in \(xz\) plane) at different load stages

From scan A in Figure 3-38, it can be noticed that there are some pre-existing interfacial and surface cracks even before the application of load. This is mainly caused during the sample preparation, due to either shrinkage during concrete hardening, or cutting process. Different levels of voids were also visualised, including big pores and micro voids. As the load was applied, some of the initial micro-cracks were closed at scan B and D, due to the compression (see highlighted areas in Figure 3-38). At scan F (the maximum force), many vertical cracks appeared, with most of them mainly parallel to the loading direction (\(Z\)). Some of them were newly generated cracks (even through aggregates), and some were the propagation of initial micro-cracks (defects at scan A).

Similar to the sample 2, the voids and cracks at scans A, B, D, F were directly segmented (see Figure 3-39). Scan A shows the pre-existed voids and cracks. By comparing scans A and B, it can be noticed that some of the cracks actually
closed and the total volume reduced. As the load was further increased, more and more micro-cracks were generated. Finally multiple surface cracks were generated at maximum load (24kN at scan F), which corresponds to the damaged sample in Figure 3-37.

![Crack network propagation in 3D](image)

**Figure 3-39 Crack network propagation in 3D**

**Localised behaviour in sub-volumes**
A small sub-volume was cropped at each load stage, to examine the localised fracture features. Figure 3-40 shows the local area under 10kN (D), 24kN (F) loads and at the final unloaded stage (G). Under 10kN (D), most damage happened at the aggregate-cement interfaces. Crack opening and closing, observed in Figure 3-38, was also indicated here. It is clear that multiple vertical cracks propagated under the maximum load 24kN (F), with most of them parallel to the load direction (Z). The interfacial cracks were fully propagated and interconnected to cause major damage. When comparing scans F and G, some of the
propagated cracks had closed and some closed cracks had re-opened after relaxation of the load. One of the interfacial cracks re-opened in shear after the remove of the load. This crack opened and then was kept intact due to the high compression load. However, it relaxed and re-opened when the load was removed. All of these internal localised features are hard to observe from conventional tests, but can be unveiled through in-situ XCT scans. This again proves that the in-situ XCT is a powerful characterisation technique.

As the 3D crack network is much more complicated than the 2D network, the cracks in a sub-volume, under different load steps (scan A, B, D, and F) are segmented and this is shown in Figure 3-41. It is noticeable that the cracks were distributed randomly and propagated in a much more complex pattern. Besides, the crack propagation direction was influenced greatly by the distribution of other phases, i.e. aggregates and cement.
Figure 3-41 Crack network propagation in a 3D sub-volume

3.4.3 3D segmentation

Phase segmentation
Similar to the sample 2, this sample at 0kN was cropped and segmented. Figure 3-42 shows the segmented phases, both separately and in a whole volume. The total cube volume is 8237 mm$^3$ with a resolution of 0.1mm. The voids were considered as empty areas. Here they are shown in 3D by different small volumes in different colours.
The volume fraction of each phase in the segmented cube is shown in Table 3-7, in which the aggregate occupies the most volume at 50.1%, followed by the cement with 48.6%. The total defects including the sample defects take the smallest value of 1.3%.

<table>
<thead>
<tr>
<th>Phase</th>
<th>Volume (mm$^3$)</th>
<th>Fraction (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aggregate</td>
<td>4123.9</td>
<td>50.1</td>
</tr>
<tr>
<td>Cement</td>
<td>4005.4</td>
<td>48.6</td>
</tr>
<tr>
<td>Voids</td>
<td>107.7</td>
<td>1.3</td>
</tr>
<tr>
<td>Total</td>
<td>8237</td>
<td>100</td>
</tr>
</tbody>
</table>

Figure 3-42 The 3D segmentation of sample 4 at 0kN
Aggregate size distribution

Figure 3-43 shows the 3D volume distribution of aggregates in sample 4. There are 117 aggregates in total, with most of them having the volume in the range of 30-50 mm\(^3\) and less than 20 mm\(^3\). This volume distribution suggests that sample 4 has more small aggregates (volume less than 1 mm\(^3\)) than sample 2, which was probably caused by sample deviation and randomness involved during segmentation. Table 3-8 shows the statistical analysis of the results. The mean volume is 35.25 mm\(^3\). The mean length and width in 3D is 6.74 and 2.83 mm, respectively. The mean value of the equivalent diameter of the segmented aggregate is 3.56 mm, with a standard deviation of 2.23 mm, which is quite close to that for the sample 2.

![Figure 3-43 3D volume distribution of aggregates in sample 4](image)

<table>
<thead>
<tr>
<th>Volume (mm(^3))</th>
<th>Equivalent Diameter (mm)</th>
<th>Length (mm)</th>
<th>Width (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>35.25</td>
<td>3.56</td>
<td>6.74</td>
</tr>
<tr>
<td>Min</td>
<td>0.03</td>
<td>0.36</td>
<td>0.76</td>
</tr>
<tr>
<td>Max</td>
<td>124.77</td>
<td>6.2</td>
<td>12.49</td>
</tr>
<tr>
<td>Standard deviation</td>
<td>30.04</td>
<td>2.23</td>
<td>7.22</td>
</tr>
</tbody>
</table>
**Voids size distribution**

As for voids, there are 33 independent defect volumes in total, which is merely 63% of the sample 2. The variability indicates that more specimens are needed (if possible) to obtain a more representative data. The 3D volume distribution of voids is shown in Figure 3-44. Table 3-9 calculates the statistical results. 3D volumes with a size smaller than 15 pixels were ignored. The mean volume is 3.26 mm$^3$, which is around double of the sample 2. It is obvious that 76% (25 out of 33) of the voids had less than the average volume. The mean values of equivalent diameter, 3D length and 3D width are 1.09mm, 2.21mm and 0.87mm respectively.

![Figure 3-44 3D volume distribution of voids in sample 4](image)

Table 3-9 Statistical analysis for voids in sample 4

<table>
<thead>
<tr>
<th></th>
<th>Volume (mm$^3$)</th>
<th>Equivalent Diameter (mm)</th>
<th>Length (mm)</th>
<th>Width (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>3.26</td>
<td>1.09</td>
<td>2.21</td>
<td>0.87</td>
</tr>
<tr>
<td>Min</td>
<td>0.02</td>
<td>0.31</td>
<td>0.59</td>
<td>0.15</td>
</tr>
<tr>
<td>Max</td>
<td>27.76</td>
<td>3.76</td>
<td>10.06</td>
<td>3.41</td>
</tr>
<tr>
<td>Standard deviation</td>
<td>7.43</td>
<td>1.02</td>
<td>5.3</td>
<td>0.76</td>
</tr>
</tbody>
</table>
3.5 Summary

Three in-situ X-ray computed tomography (XCT) experiments were conducted under compression, including a Brazilian-like compression on a 40mm cube, a monotonic compression and a cyclic compression on 20mm cubes.

After a brief introduction of the XCT characterisation technique, the procedures for the in-situ test, reconstruction and segmentation were explained in detail through the first benchmark test, with the loading concentrated on 19% of the sample cross-sectional area. The screw-driven loading system (DEBEN) was used to maintain quasi-static loading conditions. The loading curve was corrected using a digital volume correlation technique, which was more realistic. Two loading points were segmented, without load and under maximum load, to illustrate the 3D distribution of different phases (aggregate and cement, as well as voids and cracks) in the concrete.

The two 20mm cubes were cropped and in-situ scanned under monotonic compression and cyclic compression. The fracture features were characterised and visualised through 2D tomography images and 3D volumes. The sub-volume micro-cracking showed the realistic 3D damage evolution between two aggregates. The crack propagation, as well as the voids and cracks distribution, was unveiled throughout the loading steps. The evolution of volume fraction of voids and cracks, during the loading history, shows that the total volume of voids and cracks first reduced due to compression, then gradually expanded due to newly formed cracks. The CTZ width between crack and phases in concrete (i.e. aggregate and cement) and the ITZ thickness between aggregate and cement were measured directly from the XCT images.

Finally, the detailed distribution of aggregate and voids in the concrete samples was presented, which can be used for generating random concrete models (Yin et al., 2013; Wang et al., 2015b). The comparison of statistical analyses of the sample 2 and the sample 4 shows that there exists big sample deviation. However, the overall equivalent parameters of aggregates and voids show good agreement,
as they were cut from a same batch of concrete. The segmented 3D imaging models will be used for image based FE simulations in the following chapters.
Chapter 4

MICRO-INDENTATION AND HOMOGENISATION

This chapter outlines the technique used to determine some of the material parameters which will be used for later validation of the image based modelling results. More specifically, the micro-indentation test was used to estimate the Young’s modulus of the aggregate and cement. Moreover, the numerical homogenisation method was used to calculate the effective elastic properties of the concrete cube.

4.1 Micro-indentation test

The micro-indentation test was used to measure the material properties of the aggregate and the cement in the concrete. The standard procedure was applied, including sectioning, resin embedding, grinding, polishing and the final micro-indentation. This is explained in the following sections.

4.1.1 Sample preparation

Two concrete specimens of 20×10×10 mm³ and 20×20×10 mm³ were cut from the same 40 mm concrete cube (same to the sample 2 and 4 used in the previous Chapter). They were then embedded in cylindrical moulding resins of 20 mm height and 30mm diameter for the ease of grinding and polishing.

Indentation test results are greatly affected by the flatness of the sample surfaces. Therefore, the specimens were prepared by very fine grinding and polishing processes, using silicon carbide abrasive papers and diamond particles of suspensions up to 1μm. The automatic grinding and polishing machine shown in
Figure 4-1 was used. Coarse paper of 106 μm (P120 on the European P-grade) was first used, followed by 25.8 μm (P600), 15.3 μm (P1200) and 6.5 μm (P2400). Kemet diamond suspension liquids of 6 μm and 1 μm were then used. Finally, the specimens were cleaned by alcohol and distilled water to remove the dust and diamond particles that might have been left in the voids or porous areas. The final prepared specimens are shown in Figure 4-2.

![Figure 4-1 The automatic grinding and polishing machine](image1)

![Figure 4-2 Concrete specimens used for the micro-indentation test](image2)

### 4.1.2 Micro-indentation test

The CSM micro-indentation tester (CSM, 2010), with the Vickers diamond indenter, in the School of Materials at the University of Manchester, was used. Figure 4-3 shows the tester and its control system.
The micro-indentation test involves the following steps (CSM, 2010):

1. Place the sample under the measurement head;
2. Choose the indentation area using the system microscope;
3. Adjust the depth offset and make a trial indent with a small load to test the standard position of the surface;
4. Move to a nearby position and setup the measurement configurations; either a standard single indent or serial matrix tests can be assigned;
5. Start the indentation measurements and analyse the results.

All the tests in this study used a constant linear loading rate until the force of the indenter reached a specified maximum value. Then the load was held for 10s before unloading at the same rate. After unloading the specimen was moved to the next programmed point. The distance between two adjacent points was set according to the indentation results, in order to avoid possible overlapping of the affected areas. Both aggregate and cement areas in the two specimens were selected. Different aggregate grains and cement locations were tested. Also different peak forces, which relate to different indentation depths, were used to determine the Young’s modulus for the aggregates and cement.

The Oliver and Pharr method (1992) was used to calculate the Young’s modulus. A typical force-depth hysteresis curve of the micro-indentation testing is shown in Figure 4-4. Each indentation test consists of three steps. Firstly, the indenter is
gradually moved into contact with the specimen surface, and then a compression force is applied, which includes both elastic deformation and plastic deformation. Secondly, the applied load is held for a specific time at the maximum force. Finally, when the unloading is started, the recovery of the elastic deformation is calculated by analysing the unloading data, which leads to the determination of the Young’s modulus (E) as well as hardness of the test area. Details of the theoretical background and methodology have been reviewed in literature (Trtik and Bartos, 1999; Zhu and Bartos, 2000).

Figure 4-4 Typical indentation force-depth curve

Briefly, the estimated indentation modulus $E_{IT}$ is determined using Equations (4-1) and (4-2):

$$E_{IT} = \frac{1 - \mu_s^2}{\frac{1}{E_r} - \frac{1 - \mu_i^2}{E_i}}$$  \hspace{1cm} (4-1)

where $E_i$=1141 GPa represents the Young’s modulus of the indenter; $\mu_i$= 0.07 represents the Poisson’s ratio of the indenter; $\mu_s$=0.2 represents the estimated Poisson’s ratio of the sample; $E_r$ is a reduced Young’s modulus defined by

$$E_r = \frac{\sqrt{\pi}}{2} \frac{S}{\sqrt{A}}$$  \hspace{1cm} (4-2)
where $S$ is the contact stiffness at $F_{\text{max}}$, and $S = dF_{\text{max}}/dh_{\text{max}}$. $A$ represents the projected contact area and $A = f(h)$ (CSM, 2010).

### 4.1.3 Results

Figure 4-5 shows the force-depth curve and indentation mark under 5N. An elastic response curve with no clear indent notch, except for fractured surfaces, was found. Thus the indent force values for the aggregate were targeted as 1N, 0.8N, 0.5N, 0.3N and 0.1N.

In Figure 4-6, very different indentation marks were found in the same local area of an aggregate under 0.1N. They were caused by different minerals (such as quartz, feldspar and biotite etc.) in this local area. The quartz has a Mohs hardness of 7, which is nearly 3 times of biotite with a Mohs hardness of 2.5 to 3. The values can be averaged to obtain a mean value.
Chapter 4 Micro-Indentation and Homogenisation

Indentation points near holes are carefully identified and excluded from calculations, such as the example in the cement shown in Figure 4-7, because serial indentations were applied.

Finally, two examples of ready to use indents, for cement and aggregate under 0.3N, are shown in Figure 4-8. The indentation marks are very clear and have less damaged areas around them, which is sufficient to give good estimations of Young’s modulus for the tested area. The corresponding force-depth curves are shown in Figure 4-9. A much higher elastic deformation and lower total deformation (less than 25%) was observed in the aggregate than in the cement under 0.3N. This corresponds to a higher elastic modulus of the aggregate.
According to the indentation results, shown in Table 4-1, and the aforementioned analysis of indentation marks, the value of the Young’s modulus for cement and aggregate are taken as the average values for all available tests: $E_c = 13.6 \text{ GPa}$ and $E_a = 51 \text{ GPa}$ respectively. For Portland cement, the elastic modulus is normally in the range of 14GPa to 40GPa. For quartz and biotite, the elastic modulus is in the order of 70GPa and 40GPa, which suggest that the estimated 51GPa for aggregate is reasonable.
Table 4-1 Estimation of Young’s modulus for aggregate and cement under different indentation forces

<table>
<thead>
<tr>
<th>Maximum Force (N)</th>
<th>0.1</th>
<th>0.3</th>
<th>0.5</th>
<th>0.8</th>
<th>1</th>
<th>Average</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_a$ for aggregate (GPa)</td>
<td>Mean</td>
<td>50.6</td>
<td>60.0</td>
<td>53.8</td>
<td>41.7</td>
<td>48.8</td>
</tr>
<tr>
<td></td>
<td>Standard deviation</td>
<td>16.7</td>
<td>4.9</td>
<td>13.9</td>
<td>10.8</td>
<td>8.4</td>
</tr>
<tr>
<td>$E_c$ for cement (GPa)</td>
<td>Mean</td>
<td>12.0</td>
<td>16.2</td>
<td>16.2</td>
<td>13.3</td>
<td>10.3</td>
</tr>
<tr>
<td></td>
<td>Standard deviation</td>
<td>3.4</td>
<td>2.5</td>
<td>4.3</td>
<td>2.7</td>
<td>2.2</td>
</tr>
</tbody>
</table>

With the Young’s modulus and the volume fractions of aggregate ($V_F_a$) and cement ($V_F_c$) known in the concrete specimen, the lower and upper limits of Young’s modulus of the concrete cube can be estimated by the rule of mixtures (bounding methods), e.g. Reuss and Voigt rules (Hill, 1952). The upper-bound $E_{upper}$ is calculated as:

$$E_{upper} = E_a \cdot V_F_a + E_c \cdot V_F_c$$  \hspace{1cm} (4-3)

And the lower-bound $E_{lower}$ is calculated as:

$$\frac{1}{E_{lower}} = \frac{V_F_a}{E_a} + \frac{V_F_c}{E_c}$$  \hspace{1cm} (4-4)

where $E_a$ represent the Young’s modulus of aggregate;

$E_c$ represent the Young’s modulus of cement;

$E_{upper}$ represent the Young’s modulus of concrete upper bound;

$E_{lower}$ represent the Young’s modulus of concrete lower bound.

Using Equation 4-3 and 4-4, the estimated $E_{upper}$ and $E_{lower}$ for the 40mm cube are 32GPa and 22GPa. For the sample 2 and the sample 4 (20mm), they are 34 GPa and 23GPa, and 32 GPa and 22GPa, respectively.
4.2 Homogenisation

4.2.1 Methodology
As reviewed in Chapter 2, various multi-scale methods have been developed to model composite materials. One of them is homogenisation based modelling, where the composites are simulated at two scales: the global length scale of the order of the size of the structure and the local length scale proportional to the wavelength of the variation of the micro-structure (Oller, 2014). When the material’s internal structure is periodic, the representative unitary volume of this periodicity is called a unit cell (or representative volume element, RVE).

The technique of using asymptotic homogenisation along with periodic boundary conditions, is one of the most effective procedures in finite element analysis to obtain an effective homogenised stiffness matrix (Jansson, 1992; Song and Youn, 2006; Li, 2008; Sharma et al., 2014). In this technique, six loading cases are analysed using six boundary conditions, to get the averaged response. The equivalent homogeneous moduli of the concrete can then be determined and used to validate FE simulations. These techniques were used in this study.

Asymptotic homogenisation
Consider a periodic nonlinear elastic inhomogeneous body $V$ (see Figure 4-10), which comprises two constituents: the global length scale $L$ and a local length scale $l$. Constraint $U$, body forces $f$ and external tractions $T$ are applied.
The size of the RVE (domain $Y$) is assumed to be much smaller than the size of the body, thus:

$$\beta = \frac{l}{L} \ll 1$$  \hspace{1cm} (4-5)

The global length coordinate $x_i$ for the body, and the local system $y_i$ for the RVE, are related by (Jansson, 1992; Sharma et al., 2013b)

$$y_i = \frac{x_i}{\beta}$$  \hspace{1cm} (4-6)

where $\beta$ is the scaling factor between the two length scales.

The generalized Hooke’s law, equilibrium equations and strain-displacement relations, can be written as:

$$\sigma_{ij} = C_{ijkl} \varepsilon_{kl}$$  \hspace{1cm} (4-7)

$$\sigma_{ij,j} + f_i = 0 \hspace{.5cm} in \hspace{.5cm} V$$  \hspace{1cm} (4-8)

$$\varepsilon_{kl} = \frac{1}{2}(u_{kl} + u_{lk})$$  \hspace{1cm} (4-9)

where $\sigma_{ij}$ is the stress tensor, $\varepsilon_{kl}$ is the strain tensor, $C_{ijkl}$ is the material stiffness matrix, and $f_i$ is the body force per unit volume.
The boundary conditions are:

\[ \sigma_{ij} n_j = \bar{T}_i \quad \text{on} \quad S_{\sigma} \quad \text{(4-10)} \]

\[ u_i = \bar{u}_i \quad \text{on} \quad S_u \quad \text{(4-11)} \]

where \( n_j \) is the unit normal vector on the boundary, \( \bar{T}_i \) is the prescribed traction, \( u_i \) is the displacement, and \( \bar{u}_i \) is the displacement prescribed on the boundary.

The global displacement field \( u_i \) is assumed to be an asymptotic expansion with respect to parameter \( \delta \):

\[ u_i(x, y, \delta) = u^0_i(x, y) + \delta u^1_i(x, y) + \delta^2 u^2_i(x, y) + \cdots \quad \text{(4-12)} \]

where \( u^0_i(x, y) \), \( u^1_i(x, y) \), \( u^2_i(x, y) \) are slowly varying functions in \( x_i \), due to the restriction of the loading and periodic functions in \( y_i \), governed by the periodicity of the micro-structure.

The strains \( \epsilon_{ij} \) are functions of \( u_i, x, \) and \( y \), and can be expanded as:

\[ \epsilon_{ij} = \frac{1}{\delta} \epsilon^{-1}_{ij} + \epsilon^0_{ij} + \delta \epsilon^1_{ij} + \cdots \quad \text{(4-13)} \]

where \( \epsilon_{ij} \) are the strains and can be expressed as:

\[ \epsilon^{-1}_{ij} = \frac{1}{2} \left( \frac{\partial u^0_i}{\partial y_j} + \frac{\partial u^0_j}{\partial y_i} \right) \]

\[ \epsilon^0_{ij} = \frac{1}{2} \left( \frac{\partial u^1_i}{\partial x_j} + \frac{\partial u^1_j}{\partial x_i} + \frac{\partial u^1_i}{\partial y_j} + \frac{\partial u^1_j}{\partial y_i} \right) \quad \text{(4-14)} \]

\[ \epsilon^1_{ij} = \frac{1}{2} \left( \frac{\partial u^2_i}{\partial x_j} + \frac{\partial u^2_j}{\partial x_i} + \frac{\partial u^2_i}{\partial y_j} + \frac{\partial u^2_j}{\partial y_i} \right) \]

The stress from Equation (4-7) can now be written as

\[ \sigma_{ij} = \frac{1}{\delta} \sigma^{-1}_{ij} + \sigma^0_{ij} + \delta \sigma^1_{ij} + \cdots \quad \text{(4-15)} \]
Chapter 4 Micro-Indentation and Homogenisation

where

\[ \sigma_{ij}^{-1} = C_{ijkl} \varepsilon_{kl}^{-1} \]
\[ \sigma_{ij}^{0} = C_{ijkl} \varepsilon_{kl}^{0} \]  \hspace{1cm} (4-16)
\[ \sigma_{ij}^{1} = C_{ijkl} \varepsilon_{kl}^{1} \]

Combining Equations (4-7) and (4-8) and using the above forms, yields the following equation (Song and Youn, 2006; Sharma, 2012)

\[ < \sigma_{ij} > = C_{ijkl} + C_{ijmn} \frac{\partial X_{kl}^{m}}{\partial y_{n}} \varepsilon_{kl} \]  \hspace{1cm} (4-17)

Here \( X_{mn}^{kl} \) represents the deformation modes of the RVE and is a periodic function of domain \( Y \). The constitutive relations of the asymptotic homogenisation can then be written as:

\[ < \sigma_{ij} > = \frac{1}{V_{e}} \int_{V_{e}} \sigma_{ij}(x, y) dV_{e} = C_{ijkl}^{H} < \varepsilon_{ij} > \]  \hspace{1cm} (4-18)

where \( C_{ijkl}^{H} \) are the equivalent homogenised stiffness coefficients, \( < \sigma_{ij} > \) is the volume averaged stress, \( V_{e} \) is the volume of the element, and \( < \varepsilon_{ij} > \) are the volume averaged strains given by following expression:

\[ < \varepsilon_{ij} > = \frac{1}{V_{e}} \int_{V_{e}} \varepsilon_{ij}(x, y) dV_{e} \]  \hspace{1cm} (4-19)

For the concrete, the averaged strains \( < \varepsilon_{ij} > \) are divided into aggregate and cement parts:

\[ < \varepsilon_{ij} > = \frac{1}{V} \left[ \int_{V_{a}} \varepsilon_{ij}^{agg}(x, y) dV_{a} + \int_{V_{c}} \varepsilon_{ij}^{cem}(x, y) dV_{c} \right] \]  \hspace{1cm} (4-20)

where \( V_{a} \) and \( V_{c} \) are the volumes of the aggregate and the cement in the RVE.

**Periodic boundary conditions**

From the principle of symmetries, which state that symmetrical stimuli result in symmetric response, and anti-symmetric stimuli produce anti-symmetric...
response, the periodic boundary conditions were imposed on the RVEs. The individual load cases, expressed in terms of micro-stresses \((e_{11}, e_{22}, e_{33}, \gamma_{23}, \gamma_{13}, \gamma_{12})\), are applied to consider the reflection symmetries of the \(x\), \(y\) and \(z\) planes (Torquato, 2002; Sharma et al., 2013b; Sharma et al., 2014). Consider a 3D specimen with dimensions of \(b_{x}, b_{y}, b_{z}\), for \(x, y\) and \(z\) axes.

For normal loading conditions, the boundary conditions for two opposite faces of the RVE are applied; see equation (4-21). For example, when \(\sigma_{11}\) is applied, \(e_{11}\) is the associated degree of freedom at face \(x=b_{x}\); in the meantime, \(e_{22}\) and \(e_{33}\) are kept free. Similarly, for \(\sigma_{22}\) and \(\sigma_{33}\), the associated degrees of freedom are \(e_{22}\) and \(e_{33}\), at faces of \(y=b_{y}\) and \(z=b_{z}\) respectively, and the other strains are kept free.

\[
\begin{align*}
 u|_{x=0} &= 0 \quad \text{and} \quad u|_{x=b_{x}} = b_{x}e_{11} \\
 v|_{y=0} &= 0 \quad \text{and} \quad v|_{y=b_{y}} = b_{y}e_{22} \quad (4-21) \\
 w|_{z=0} &= 0 \quad \text{and} \quad w|_{z=b_{z}} = b_{z}e_{33}
\end{align*}
\]

where \(u\), \(v\) and \(w\) are displacements of each node in \(x\), \(y\) and \(z\) directions.

For the implementation of shear loading conditions, the corresponding Equations are in (4-22), (4-23) and (4-24).

\[
\begin{align*}
 u|_{x=0} &= u|_{x=b_{x}} = 0 \\
 u|_{y=0} &= w|_{y=0} = u|_{y=b_{y}} = w|_{y=b_{y}} = 0 \quad (4-22) \\
 u|_{z=0} &= v|_{z=0} = u|_{z=b_{z}} = 0 \quad \text{and} \quad v|_{z=b_{z}} = b_{z}\gamma_{23}
\end{align*}
\]

\[
\begin{align*}
 v|_{x=0} &= w|_{x=0} = v|_{x=b_{x}} = w|_{x=b_{x}} = 0 \\
 v|_{y=0} &= v|_{y=b_{y}} = 0 \quad (4-23) \\
 u|_{z=0} &= v|_{z=0} = v|_{z=b_{z}} = 0 \quad \text{and} \quad u|_{z=b_{z}} = b_{z}\gamma_{13}
\end{align*}
\]

\[
\begin{align*}
 v|_{x=0} &= w|_{x=0} = v|_{x=b_{x}} = w|_{x=b_{x}} = 0 \\
 u|_{y=0} &= w|_{y=0} = w|_{y=b_{y}} = 0 \quad \text{and} \quad u|_{y=b_{y}} = b_{y}\gamma_{12} \quad (4-24) \\
 w|_{z=0} &= w|_{z=b_{z}} = 0
\end{align*}
\]
4.2.2 Homogenisation analysis of the 40mm cube

The components of $C_{ijkl}^H$ (the equivalent homogenised stiffness coefficients) were obtained by the aforementioned asymptotic homogenisation along with periodic boundary conditions. The averaged Young’s moduli of 51GPa and 13.6GPa for aggregate and cement were used as input. The Poisson’s ratio was assumed as 0.2. The 3D segmented concrete cube in Chapter 3.2.4 for the Brazilian-like test was used. The commercial software Simpleware (Simpleware, 2011) was used to generate FE meshes with different sizes of RVEs (i.e. 10, 20, 30 and 37 mm cubes). To investigate the effect of the random distribution of internal phases in concrete, different realisations were used for each size: 5 for the 10 mm cube, 3 for the 20 mm cube, 2 for the 30 mm cube and 1 for the full model (37 mm cube). The reconstructed RVEs are shown in Figure 4-11.

![Figure 4-11 Reconstructed RVEs with different sizes, with colours in yellow, cyan and purple represent aggregates, cement and voids.](image)

Six individual load cases for all of the RVEs were analysed using FE analysis. Taking realisation 1 of the 10 mm RVE cube (RVE10-1) in Figure 4-11 as an example, the stress distributions for different load cases are shown in Figure 4-12. Figure 4-12a shows the stress distribution under $\sigma_{11}$ loading, with the $x=0$ face
fixed and the $x=b_x$ face loaded by a unit length displacement. Similarly, Figure 4-12b, c, d, e, and f correspond to the loading conditions of $\sigma_{22}$, $\sigma_{33}$, $\tau_{12}$, $\tau_{13}$ and $\tau_{23}$ respectively. Different load cases generate different stress distributions, and the aggregates can be clearly seen as they have higher stresses than the cement for all six load cases.

The homogenised stiffness coefficients of RVE10-1 are shown in equation (4-25). The coupling terms show that the values of extension-shear and shear-shear were far less than that of extension-extension, and hence they were ignored for further calculations.

$$C_{ijkl}^H = \begin{bmatrix}
26.77 & 6.74 & 6.73 & 0.12 & 0.48 & -0.015 \\
27.57 & 6.70 & 0.30 & 0.16 & 0.23 \\
27.10 & 0.012 & 0.17 & -0.03 \\
10.19 & 0.028 & 0.35 & - & \\
10.12 & 0.083 & - & \\
10.20 & - & - & & \\
\end{bmatrix}$$

Thus the calculated mean values of the coefficients, with associated standard deviations for 10mm RVEs, are given as:
A clear cubical symmetry was obtained for coefficients $C_{ijkl}^{H}$ of the concrete. Therefore, the engineering elastic constants of concrete were extracted. The volumetric average values for all the RVE sizes, by considering the uncertainties of the specimens, are given in Table 4-2. It is found that the engineering constants are decreasing when the RVE size increases. Thus, different RVE sizes might have different engineering elastic constants, e.g. 3.5% difference for RVE10 and RVE37.
### Table 4-2 Homogenised engineering constants with associated uncertainties

<table>
<thead>
<tr>
<th>RVE size</th>
<th>$E_{11}$ (GPa)</th>
<th>$E_{22}$ (GPa)</th>
<th>$E_{33}$ (GPa)</th>
<th>$\mu_{12}$</th>
<th>$\mu_{13}$</th>
<th>$\mu_{23}$</th>
<th>$G_{12}$ (GPa)</th>
<th>$G_{13}$ (GPa)</th>
<th>$G_{23}$ (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^3$ mm$^3$</td>
<td>24.45 ± 0.58</td>
<td>24.72 ± 0.43</td>
<td>24.91 ± 0.65</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
<td>10.11 ± 0.13</td>
<td>10.19 ± 0.20</td>
<td>10.23 ± 0.14</td>
</tr>
<tr>
<td>$20^3$ mm$^3$</td>
<td>24.19 ± 1.05</td>
<td>24.73 ± 1.08</td>
<td>24.96 ± 1.28</td>
<td>0.195</td>
<td>0.193</td>
<td>0.195</td>
<td>10.08 ± 0.47</td>
<td>10.15 ± 0.46</td>
<td>10.30 ± 0.48</td>
</tr>
<tr>
<td>$30^3$ mm$^3$</td>
<td>23.67 ± 0.35</td>
<td>24.40 ± 0.37</td>
<td>24.47 ± 0.38</td>
<td>0.194</td>
<td>0.194</td>
<td>0.195</td>
<td>9.93 ± 0.13</td>
<td>9.97 ± 0.15</td>
<td>10.15 ± 0.16</td>
</tr>
<tr>
<td>$37^3$ mm$^3$</td>
<td>23.58</td>
<td>24.22</td>
<td>24.38</td>
<td>0.194</td>
<td>0.193</td>
<td>0.194</td>
<td>9.92</td>
<td>9.95</td>
<td>10.11</td>
</tr>
<tr>
<td>EHEP</td>
<td>23.67 ± 0.21</td>
<td>24.33 ± 0.22</td>
<td>24.47 ± 0.24</td>
<td>0.194</td>
<td>0.193</td>
<td>0.194</td>
<td>9.94 ± 0.08</td>
<td>9.98 ± 0.09</td>
<td>10.14 ± 0.09</td>
</tr>
</tbody>
</table>
Furthermore, the volumetric average of all the RVEs was calculated (e.g. \( E_{11} \) in Equation (4-27) and considered as the effective homogenised elastic properties (EHEP) for concrete. This gives the estimated values of normal elastic modulus, Poisson’s ratio and shear modulus of concrete, as 24.16GPa, 0.194 and 10.02GPa respectively. The calculated normal elastic modulus lies in the range of 23-34GPa from the micro-indentation tests. As the elastic constants differ by a very small amount, it is reasonable to consider concrete as isotropic material for the design of structures.

\[
E_{HEP} = \frac{V_1 E_{11}^1 + V_2 E_{11}^2 + V_3 E_{11}^3 + \cdots}{V_1 + V_2 + V_3 + \cdots} \tag{4-27}
\]

4.3 Summary

The micro-indentation technique was introduced and used to determine some of the material properties of the concrete specimen, which will be used later for XCT image-based simulations. Following the standard micro-indentation test procedure, two concrete specimens were tested. The average value of Young’s modulus of the aggregate and the cement were estimated as 51GPa and 13.6GPa, respectively, and the estimations of the upper and lower bounds for the whole concrete cube were 34GPa and 22GPa, respectively.

The second technique used in this chapter was image based asymptotic homogenisation along with periodic boundary conditions. Different sized RVEs were constructed to conduct FE elastic simulations. Six loading cases were analysed using six boundary conditions to get the averaged responses. A small deviation of different RVE sizes, as well as different realisations for a specific size, was found. Thus the effective homogenised elastic properties for concrete were calculated as the volume averaged values for all the RVEs. The calculated elastic modulus, Poisson’s ratio and shear modulus of concrete were 24.16GPa, 0.194 and 10.02GPa, respectively. These values will be used to validate 3D
image-based FE modelling results in the following chapters, especially the elastic stage of the force-displacement curves.
Chapter Five

2D XCT-IMAGE BASED MODELLING

This chapter presents the results of the 2D XCT-image based numerical simulations. It is based upon the segmented image model of the Brazilian-like in-situ XCT test described in Chapter 3. Following several image processing operations, the cross-sections of the 3D image model were transformed into FE meshes. The zigzagged boundaries from pixel-based FE meshes were smoothed. 2D meso-scale models incorporating specially designed cohesive interface elements (CIEs) were generated. An efficient algorithm was coded in MATLAB for transforming the 2D images into FE meshes. The FE simulations with parametric studies were carried out using ABAQUS. A size-effect study under uniaxial tension was also attempted. Finally, the 2D FE models were simulated under uniaxial compression.

The first significance of doing 2D research rather than 3D is that the topology in 2D is much more simple and the insertion of CIEs is more straightforward, which are helpful for programming both in 2D and 3D. Furthermore, the pixel-based 3D modelling method (Huang et al., 2015) uses 2D slice information to construct 3D model, which can be compared with the 2D statistical simulations (simulating all the slices in the direction) that conducted in this Chapter.

5.1 Generation of 2D finite element meshes

The segmented 37.2 mm concrete cube from the Brazilian-like in-situ XCT test is shown in Figure 5-1. The locations of a few representative cross-sections are highlighted, as these are studied later. There are 373 cross-sections in the $x/y/z$
planes. Cross-section 1 represents surface 1 in the $xy$ plane and 40, 100 and 240 are the corresponding cross-sections in $yz$ plane.

Figure 5-1 Segmented X-ray tomography of the cube with the matrix in grey, the aggregates in black and the voids in white.

5.1.1 Image processing

Figure 5-2a shows a representative virtual $xy$ slice (cross-section 1 in Figure 5-1). In this segmented image, the pixels representing the aggregates, cement and voids were assigned with unique grey-scale values, i.e., 1 for aggregates, 2 for cement and 3 for voids. There are 372 pixels in each direction and the total length is 37.2 mm, thus each pixel length is 0.1 mm. Further image processing operations were conducted to condition the subsequent mesh. Phase regions of one pixel width (examples highlighted by red circles in Figure 5-2a) would unnecessarily increase the number of finite elements and could lead to numerical difficulties in the FE analysis (Sharma et al., 2013b; Ren et al., 2015). The grey levels of these regions were thus changed to be consistent with their surrounding values. The processed image of cross-section 1 is shown in Figure 5-2b.
Figure 5-2 Segmented virtual $xy$ slice (cross-section 1) (a) before and (b) after image processing to improve the FE meshing. The black, grey and white regions represent aggregates, cement and voids, respectively. The insets show magnified regions.

5.1.2 Initial mesh generation

A 2D slice comprises an array of square pixels. Figure 5-3a shows a small part of cross-section 1 (which is shown in Figure 5-2b). Each pixel area can be modelled by a quadrilateral element in the FE mesh. The resultant mesh is shown in Figure 5-3b, in which the boundaries between two phases are zigzagged. This situation is caused by image digitisation and does not represent the real material interfaces well. In addition, the stress concentration at the corner points may lead to numerical difficulties in the FE simulations. Therefore, these inter-phase boundaries were smoothed by dividing the corner elements into two triangles and assigning adjacent phase values (see Figure 5-3c). After mesh smoothing, the volume fraction of the voids changes from 0.47% to 0.50%, 50.72% to 51.84% for aggregates, and 48.81% to 47.66% for cement. These small changes are considered acceptable.
5.1.3 Insertion of cohesive interface elements

In order to simulate the fracture process, four-noded cohesive CIEs having zero in-plane thickness were inserted into all over the smoothed initial mesh to represent potential cracks. The detailed CIE insertion procedure devised for homogeneous materials in (Yang et al., 2009), was extended to account for multiple phases and interfaces. Three sets of CIEs with different traction-separation laws were inserted, namely, CIE_AGG within the aggregate, CIE_CEM within the cement, and CIE_INT on the aggregate-cement interfaces. As the aggregates have a much higher strength than the cement and the interfaces in normal concrete, here cracks were prevented from initiating inside the aggregates by assuming elastic behaviour without damage to CIE_AGG. However, it is possible to model crack propagation through aggregates (e.g. lightweight concrete) by assigning damage properties to CIE_AGG.

The main 2D CIEs insertion procedure was organized as follows:
(1) Import the 2D initial mesh and identify the nodes and solid element types with different phases, such as CPS3 and CPS4R for aggregates and cement;
(2) Store the topological (node, edge, face, element) connectivity within all elements, and mark nodes according to the positions (such as nodes in aggregate as 1, in cement as 2, and on interfaces as 3);
(3) Insert new nodes. For every single node, N numbers of new nodes are generated to replace the original one when this node connects to N number of solid elements (see Figure 5-4 for an example). The new generated nodes have the same coordinates;

(4) Update the topological structures in step 2, including the position marks of the new nodes;

(5) Generate and mark the new CIEs. The CIEs are built by connecting four nodes (generated in step 3) between the two neighbouring solid elements. The original solid elements are no longer connected by shared nodes, which instead are linked by those newly inserted zero thickness CIEs (in Figure 5-4c, the CIE is exaggerated for clarity reason). The three types of CIEs are distinguished by their positions (in aggregates, cement, or on interfaces);

(6) Export the mesh information. The nodes and element sets relating to the different phases are exported in the format of an ABAQUS input file.

![Initial mesh around one node](a) Mesh after insertion (b) CIE (c) Zero thickness

Figure 5-4 Insertion of CIEs

The final 2D FE mesh based on the XCT image after the insertion of the CIEs is shown in Figure 5-5. It has 357,324 nodes and 291,875 elements including 141,505 plane stress elements (CPS3 and CPS4R for triangle and quadrilateral elements) and 150,370 CIEs. The CIE_INT elements are shown as red lines.
5.2 Model parameters

Following the method introduced in section 5.1, 373 2D meso-scale FE meshes for 373 cross-sections were constructed, including the first one in the $xy$ plane (see Figure 5-5) and 372 slices in the $yz$ plane. The mesh size was 37.2 mm $\times$ 37.2 mm. The 2D solid elements (CPS3 and CPS4R) used for the aggregates and the cement were assumed to behave linear elastically. Linear tension/shear softening laws were used to model the CIEs, with quadratic nominal stress initiation criterion and linear damage evolution criterion (Yang et al., 2009). For comparison, the same material properties as in (López et al., 2008a) were used here. They are listed in Table 5-1. Due to the lack of experimental data, the shear fracture properties (elastic stiffness, cohesive strength and fracture energy) were assumed to be the same as the normal ones (e.g. $t_s = t_l = t_n$).
Uniaxial tension tests were simulated first. By default, the meshes were fixed at the left boundary and were subjected to a uniformly distributed displacement at the right boundary. The displacement-controlled loading scheme was used. All analyses were ended at a displacement \( d = 0.2 \) mm or a strain \( \varepsilon = 0.0054 \). The ABAQUS/Explicit module was used to solve the nonlinear equation systems with a step time of 0.01s, which was found to be sufficiently long for the quasi-static loading conditions.

As the ABAQUS/Explicit solver was used, the computational time could be reduced by parallel computing. The acceleration ratio was investigated on a supercomputer, with two Intel Xeon CPUs @2.8GHz of 24 cores in total and 24GB RAM. From Figure 5-6, when more CPU cores were assigned, the computing time was reduced significantly. With only two cores, it required nearly 19 hours for one 2D simulation, but the time reduced to 2.25 hours with 24 cores. From the curve, it can be noticed that the convergence time is around 12 cores of 3.5 hours for one simulation, which achieved a fair balance between use of computing time and the cost.

### Table 5-1 Material properties

<table>
<thead>
<tr>
<th></th>
<th>Young’s modulus ( E ) (MPa)</th>
<th>Poisson’s ratio ( \mu )</th>
<th>Density ( \rho ) (kg/m(^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>2500</td>
<td>/</td>
<td>/</td>
<td>/</td>
</tr>
<tr>
<td>Cement</td>
<td>25000</td>
<td>0.2</td>
<td>2200</td>
<td>/</td>
<td>/</td>
<td>/</td>
</tr>
<tr>
<td>CIE_AGG</td>
<td>/</td>
<td>/</td>
<td>2500</td>
<td>( 10^6 )</td>
<td>/</td>
<td>/</td>
</tr>
<tr>
<td>CIE_CEM</td>
<td>/</td>
<td>/</td>
<td>2200</td>
<td>( 10^6 )</td>
<td>6</td>
<td>0.06</td>
</tr>
<tr>
<td>CIE_INT</td>
<td>/</td>
<td>/</td>
<td>2200</td>
<td>( 10^6 )</td>
<td>3</td>
<td>0.03</td>
</tr>
</tbody>
</table>
5.3 Typical uniaxial tension results

5.3.1 Stress-displacement behaviour

Figure 5-7 shows the stress-displacement (σ-d) curve for cross-section 1 under uniaxial tension in the horizontal (X) direction, along with the experimental results obtained by (Hordijk, 1992) and a simulation of a 2D meso-structure (López et al., 2008a). The assumed micro-structure of the reference simulation (López et al., 2008a) is shown in Figure 5-8. The stress σ is calculated by dividing the total nodal reaction force of all the nodes on the left boundary by the specimen length (X axis). It can be seen that the peak loads and the post-peak softening responses are broadly similar for all three curves. However, the curves in Figure 5-7 should not be compared quantitatively, as they describe specimens of different sizes and phase proportions.
Figure 5-7 \(\sigma-d\) curves under uniaxial tension (volume fractions of aggregates are 52\%, 50\% and 45\% for the present study, experiment (Hordijk, 1992) and reference simulation (López et al., 2008a), respectively).

5.3.2 Micro-crack propagation

Figure 5-9 illustrates the initiation and propagation of micro-cracks before peak load (points marked A, B, C and D in Figure 5-7), which are represented by the CIEs having a scalar damage variable (SDEG) greater than 0.9. It should be noted that SDEG=1.0 means complete failure. A displacement scale factor (DSF) 10 was used in all deformed crack patterns for clarity, unless specified otherwise. Figure 5-9a shows that a few micro-cracks initiate on the aggregate-cement interfaces at a low stress \(\sigma=2.36\) MPa (Point A in Figure 5-7). As the stress increases, more and more micro-cracks appear, with most of them approximately
perpendicular to the loading direction. Figure 5-9b shows a complex micro-crack pattern in the nonlinear stage ($\sigma=3.03$ MPa at Point B). When it approaches the peak load ($\sigma=3.34$ MPa at Point C), the micro-crack pattern in Figure 5-9c looks similar to that at the peak load ($\sigma=3.36$ MPa at point D). The simulations in Figure 5-9 suggest that a large number of micro-cracks initiate very quickly at an early stage of loading, and that the micro-crack pattern gradually becomes stable in the nonlinear pre-peak stage. It can also be seen that before the peak load is reached, the micro-cracks are not connected to form any dominant macro-cracks. This is because most of them lie on the aggregate-cement interfaces due to the relatively low cohesive strength (3 MPa), and only a small number of them are inside the cement due to its higher cohesive strength (6 MPa). The simulation illustrates that the approach of pre-inserting CIEs is very flexible and powerful for modelling complex fracture processes.
Figure 5-9 The evolution of pre-peak micro-cracking for cross-section 1 at various stages in Figure 5-7. (For clarity the 3 phases are not shown.)

5.3.3 Macro-crack propagation

As is evident from Figure 5-10, the peak load (strength) is followed by the macro-crack propagation process (points marked D, E, F and G in Figure 5-7). It can be seen that macro-cracking is not evident at the peak load (Figure 5-10a). As the displacement further increases, some aggregate-cement interfacial cracks continue to propagate and gradually coalesce with newly formed cracks in the cement phase (Figure 5-10 b and c). Ultimately, the specimen fails with two main macro-cracks. It should be noted that the micro-cracks in Figure 5-9 still exist, but they are not shown in Figure 5-10 because their widths are much smaller than those of the two macro-cracks. The maximum crack opening is 0.0042 mm for point D and 0.0778 mm for point G.
5.3.4 Localised fracture

Figure 5-11 shows the sequence of crack propagation events for a localised region (the yellow region highlighted in Figure 5-10). It shows that the fracture starts from aggregate-cement interfacial micro-cracks. When two interfacial cracks occur around adjacent aggregates, a crack inside the cement initiates which bridges the interfacial cracks so that a connected crack path is formed. Meanwhile, some nearby cracks become unloaded and closed. This again demonstrates the powerful capability of the pre-inserting CIE method for
modelling complex fracture sequences and for elucidating the fundamental mechanisms.

\[ d = 0.0087 \text{mm} \quad (D) \]
\[ d = 0.0116 \text{mm} \quad (E) \]
\[ d = 0.0149 \text{mm} \quad (F) \]
\[ d = 0.0229 \text{mm} \quad (G) \]

Figure 5-11 Sequence showing the cracking propagation leading up to failure for a localised region, \( DSF = 20 \).

### 5.4 Effects of mesh type and inter-phase boundaries

The FE mesh of cross-section 1 in Figure 5-5 mainly consists of quadrilateral elements (CPS4R). Only the inter-phase boundaries are smoothed, using right-angled isosceles triangle elements. To investigate the effect of element types, HyperMesh (HyperWorks, 2013) was used to generate a mesh solely with equilateral triangle elements (CPS3). Meanwhile, the mesh before smoothing
(see Figure 5-3b) containing only quadrilateral elements was also modelled. Figure 5-12a and Figure 5-12b show the same local region modelled by CPS3 elements only and CPS4R elements only.

![Comparison of mesh types](image)

(a) CPS3 elements only  (b) CPS4R elements only

Figure 5-12 Comparison of mesh types.

The predicted stress-strain ($\sigma$-$\varepsilon$) curves for the different meshes are shown in Figure 5-13. It can be seen that the results from the hybrid mesh (see Figure 5-5) and the CPS3 element only mesh are very close, whereas the mesh with only CPS4R elements predicts a tensile strength 6% larger than the other two. This could be caused by the unsmooth, zigzagged boundaries in cement elements as well as on aggregate-cement interfacial elements in Figure 5-12b. The predicted crack patterns are shown in Figure 5-14a and Figure 5-14b, respectively, which can be compared with Figure 5-10d. Two main macro-cracks occurred for all three meshes. However, the two cracks in the mesh with only CPS4R elements appear to propagate more independently than the other two. This is in line with a higher residual stress in Figure 5-13.
Figure 5-13 $\sigma$-$\varepsilon$ curves predicted from meshes with different element types.

(a) Only CPS3 elements  (b) Only CPS4R elements

Figure 5-14 Crack patterns influenced by element types ($\varepsilon=0.0021$).

5.5 Effects of loading direction (different micro-structures with the same volume fractions)

The mesh in Figure 5-5 was also simulated under uniaxial tension but in the vertical ($Y$) direction. Similarly, two main macro-cracks were predicted; however, they were more independent (see Figure 5-15). The predicted $\sigma$-$\varepsilon$ curves are shown in Figure 5-16. It can be seen that the predicted strengths of the same specimen differ about 11% (3.36 MPa and 3.80 MPa for $X$ and $Y$ loads). These differences are caused by different distributions of phases (since the same
volume fractions of each phase are maintained) under a same loading scheme.
The pre-peak elastic parts of the two curves in Figure 5-16 are identical and
independent of the phase distribution. This has also been reported in (Skarżyński
and Tejchman, 2010; Yin et al., 2013).

Figure 5-15 Typical crack pattern
for cross-section 1 under vertical
tension ($\varepsilon = 0.002$).

Figure 5-16 $\sigma$-$\varepsilon$ curves under different
tension directions.

5.6 Effects of micro-structural heterogeneity

To examine the variation in performance with micro-structural heterogeneity, the
results for various cross-sections are presented here (slice numbers 40, 100 and
240, shown in Figure 5-1). The stochastic fluctuation in phase volume fractions
and the predicted tensile strengths for the different slices are shown in Figure 5-
17. There is no evident correlation between the volume fractions of cement and
aggregates and the tensile strength. However, there is a clear trend that higher
void volume fractions lead to lower strength, indicating that the internal defects
should be minimized for optimal material design.
Figure 5-17 Phase volume fractions and predicted tensile strengths for the different cross-sections.

The predicted $\sigma$-$\varepsilon$ curves are compared in Figure 5-18, along with the final crack patterns shown in Figure 5-19 to Figure 5-21. It can be seen that in the case of two main macro-cracks (Figure 5-10d and Figure 5-19), the strength drops slowly and the residual strength is relatively high. However, the strength drops to near zero much more quickly when only one main macro-crack occurs (Figure 5-20 and Figure 5-21). This may be due to the easier formation of a weakest link in the latter case, and once formed the single crack opens much faster, whereas in the two-crack case the strong aggregates between the two cracks prevent them from bridging or linking into a single crack and this results in a higher residual load-carrying capacity. It is also demonstrated that the $\sigma$-$\varepsilon$ curves are closely correlated to the meso-scale crack propagation process, which is closely related to the heterogeneous internal meso-structures. The different load-carrying capacities and crack patterns, at different locations in the same specimen, reflect the effects of random distribution of phases of random shapes and sizes. This also demonstrates the limitations of 2D meso-scale modelling and the necessity of 3D modelling, as there exists only one crack pattern in the physical test of one specimen.
Chapter 5 2D XCT-Image Based Modelling

Figure 5-18 $\sigma$-$\varepsilon$ curves from different images.

Figure 5-19 Crack pattern of cross-section 40 ($\varepsilon=0.002$).

Figure 5-20 Crack pattern of cross-section 100 ($\varepsilon=0.002$).

Figure 5-21 Crack pattern of cross-section 240 ($\varepsilon=0.002$).

5.7 Crack pattern match of serial slices

Figure 5-22 shows the investigation of three serial slice images in the $yz$ plane. The $\sigma$-$\varepsilon$ curves in Figure 5-22a show a very fine agreement between slices 8, 9 and 10. The main macro-cracks were also matched. This illustrates that the crack patterns of the 2D simulations of serial slices were continuous in 3D. A few differences of the macro-cracks were also observed, due to the gradual change of local micro-structure.
Chapter 5 2D XCT-Image Based Modelling

5.8 Statistical analysis of predicted strengths

Figure 5-23 shows the predicted $\sigma$-\(\varepsilon\) curves from 372 images in the \(yz\) plane and the mean curve. The mean value and standard deviation (SD) of the effective strengths are 3.39 MPa and 0.32 MPa. The cross-sections near 240 (Figure 5-21) contained large voids, which resulted in much lower strengths. The scatter in the predicted strength and the softening tails reflect the different micro-structures.
Chapter 5 2D XCT-Image Based Modelling

Figure 5-23 Predicted $\sigma$-$\varepsilon$ curves of 372 images in the $yz$ plane and the mean curve

The probability density function (PDF) of the predicted strengths for 372 slices in the $yz$ plane was calculated. The best-fit Gaussian-distribution PDF curve is plotted in Figure 5-24, which can be used to evaluate structural reliability caused by material random heterogeneity (Yang et al., 2009; Su et al., 2010b).

Figure 5-24 The best-fit Gaussian-distribution PDF curve of the predicted strengths

134
Figure 5-25 shows that statistically there exists an inversely proportionate relationship between the predicted strength and the void volume fraction. It should be noted that 320 (86%) of the images have a void volume fraction less than 1%, with their predicted strength between 3.1-3.9 MPa. In the practical design, less voids involved during concrete forming process normally will generate higher tensile strength structures.

![Graph showing the relationship between predicted strength and void volume fraction](image)

Figure 5-25 The predicted strength and void volume fraction for different slices

### 5.9 Parametric study

#### 5.9.1 Control parameters of the linear cohesive law

The cohesive crack model used here is dependent on the normal/shear cohesive strengths ($t_n = t_s = t_n$) and the corresponding failure separations. The failure separations can be calculated from the fracture energy $G_F$, when the linear softening T-S law is used. So the most pronounced effects of material input come from $t_n$ and $G_F$, that are assigned to cohesive elements in CIE_INT and CIE_CEM. Parametric studies were conducted to investigate their effects using the mesh in Figure 5-5. The values in Table 5-1, namely, $t_{nc}=6$ MPa and $G_{Fc}=0.06$ N/mm for cement, and $t_{ni}=3$ MPa and $G_{Fi}=0.03$ N/mm for the aggregate-cement interfaces, were used as default values. In a parametric analysis, only one of these four parameters was varied for each simulation, with other three taking the default values.
Figure 5-26a shows the effects of varying the interfacial cohesive strength $t_{ni}$. It can be seen that the interfacial cohesive strength is the dominant factor governing the specimen strength. This is because the higher cement cohesive strength $t_{nc}=6$ MPa meant that the fracture always originated from micro-cracks on the interfaces. The effects of the interfacial fracture energy $G_{Fi}$ are shown in Figure 5-26b. It is clear that it has no significant influence on the specimen strength, but has a significant influence on the post-peak softening responses. Figure 5-26c shows that the fracture energy of the cement cohesive elements $G_{Fc}$ affects the softening stage too, but not by as much as the interfacial fracture energy. The effects of cement cohesive strength $t_{nc}$ are shown in Figure 5-26d. The specimen strength jumps from 2.7MPa for $t_{nc}=3$MPa to 3.4MPa for $t_{nc}=6$MPa, but further strengthening becomes insignificant when $t_{nc}$ is above 6 MPa. This is related to the micro-/macro-cracking processes.
Figure 5-27a and Figure 5-27b show the pre-peak micro-cracks in cement and on the interfaces for $t_{nc}=3\text{MPa}$, which can be compared with Figure 5-27c and Figure 5-27d for $t_{nc}=6\text{MPa}$ at the same loading. It is clear that when the cohesive strengths in the cement and on the interfaces are the same ($t_{nc}=t_{ni}=3\text{MPa}$), comparable numbers of micro-cracks occur in both the cement and the interfaces, whereas most of them lie on the interfaces when the cement strength is doubled. This results in quite different final macro-crack patterns, as shown in Figure 5-28a and b for $t_{nc}=3\text{MPa}$ and 12MPa. Therefore, the relative ratio of cohesive strengths in the cement and the interfaces plays an important role in the micro-cracking behaviour, which in turn affects the macro-cracking behaviour and the load-carrying capacity of structures.

![Figure 5-27 Micro-cracks propagated separately ($\varepsilon=0.0017$)](image_url)
Chapter 5 2D XCT-Image Based Modelling

Figure 5-28 Effects of cement cohesive strength on the crack pattern
$(\varepsilon=0.0021 \text{ mm})$

5.9.2 Elastic stiffness of CIEs

It is recommended in literature that the elastic stiffness of CIEs should be high enough to represent the un-cracked material, but not too high to cause numerical ill-conditioning. According to the suggestions in (López et al., 2008a), more values were examined here. The results are shown in Figure 5-29. For each curve in the diagram, the legend after the specimen size (37.2mm) is the corresponding values of CIE elastic stiffness, from $5.0E+4$ to $1.0E+6$. As the value decreases, a clear reduction of the pre-peak slope and peak value (tensile strength) is observed, which may cause incorrect predictions. A value higher than $1.0E+6$ is not acceptable for a complete FE simulation. Thus the value of $1.0E+6$ that used in all the FE simulations is reasonable.
5.9.3 Loading magnitude

The loading magnitude was also investigated. This is shown in Figure 5-30 (the step time is set to be 0.01s). An excellent agreement was reached as expected. This is mainly because of the explicit solver, which uses an automatic time incrementing scheme.

5.9.4 Boundary condition

To examine the effects of boundary conditions, two types of constraint were applied. One was simply supported constraints (constrain the X-direction to the
left-side nodes with only one node to be fixed), while the second fixed all the left-side nodes and apply displacements on the right side. The predicted $\sigma$-$d$ curve is shown in the Figure 5-31. The result shows that two types of boundary conditions make no difference. For all the 2D simulations, the fixed condition was used.

![Figure 5-31](image)

Figure 5-31 The influence of boundary conditions on the $\sigma$-$d$ curve

### 5.10 Size effect study

To investigate the size effect under uniaxial tension, different sized meshes were firstly constructed by cropping the aforementioned 2D FE mesh in Figure 5-5. One major motivation was to identify whether the mesh size of 37.2mm was representative, with respect to the particle size (5mm). Different mesh sizes (2/3/4/5/6/7 times the particle size) were selected, based on the same centre of the full mesh, both with and without voids. Then more meshes with diverse micro-structures were constructed from multiple slices in Figure 5-1. Periodic boundary conditions were used for all of the FE simulations in this section.

#### 5.10.1 Centred meshes with voids

Based on the 2D mesh of the cross-section in Figure 5-5, six meshes were cropped into 10/ 15/ 20/ 25/ 30/ 35 mm, which is equal to 2/ 3/ 4/ 5/ 6/ 7 times the average aggregate size. Table 5-2 shows the volume fraction of each phase
Chapter 5 2D XCT-Image Based Modelling

for the different mesh sizes. The volume fractions of aggregates and cement for different sizes are not varied too much; however, the voids’ volume differs largely. The locations are shown in Figure 5-32, in which the same centre microstructure was preserved. The corresponding $\sigma$-$\varepsilon$ curves are plotted in Figure 5-33. During the pre-peak linear-elastic stage, the stiffness (slope of the $\sigma$-$\varepsilon$ curve) remained identical when the size was increasing. Then the curves started to deviate once the mesh was in the nonlinear hardening stage near peak strength. A clear trend was observed, with an increase of mesh size, the increase of overall strength (peak value) became smaller; moreover, the brittleness (post-peak softening stage) first increased greatly and then gradually became stable. There is no evident size effect on the predicted strength. The meshes over 20 mm were considered to behave representatively.

Table 5-2 Volume fraction of each phase in different mesh sizes

<table>
<thead>
<tr>
<th>Volume Fraction (%)</th>
<th>Mesh size (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>10</td>
</tr>
<tr>
<td>Aggregate</td>
<td>61.50</td>
</tr>
<tr>
<td>Cement</td>
<td>36.46</td>
</tr>
<tr>
<td>Voids</td>
<td>2.04</td>
</tr>
</tbody>
</table>

Figure 5-32 Mesh locations at different sizes
As mentioned in Section 5.5, different micro-structures were considered with the same volume fractions of each phase by applying load on different axes. Table 5-3 shows the predicted tensile strength of different sized meshes under X and Y axial loads. From Table 5-3 it can be seen that the predicted strength is not as expected from literature (Nallathambi et al., 1985; Gitman et al., 2007). The size effect law is that the strength decreases as the mesh size increases. One possible reason is that the size range is not wide enough. Besides, the tensile strength is highly dependent on the heterogeneous micro-structure in the mesh. However, for all the centred mesh sizes, only one mesh was extracted for each size, which is insufficient and will be discussed later for multiple meshes. This is not statistical representative. Another possible reason relates to the voids effect. Table 5-2 illustrates that the volume fraction of voids became smaller for increased mesh size. This is because, when the mesh size is reduced, a same volume of void will have a larger effect on the tensile strength, due to the consequent larger volume fraction in a smaller mesh.
Chapter 5 2D XCT-Image Based Modelling

Table 5-3 Predicted tensile strength of different meshes under X and Y loads

<table>
<thead>
<tr>
<th>Mesh size (mm)</th>
<th>10</th>
<th>15</th>
<th>20</th>
<th>25</th>
<th>30</th>
<th>35</th>
<th>37.2</th>
</tr>
</thead>
<tbody>
<tr>
<td>X strength (MPa)</td>
<td>3.01</td>
<td>3.18</td>
<td>3.34</td>
<td>3.27</td>
<td>3.24</td>
<td>3.38</td>
<td>3.41</td>
</tr>
<tr>
<td>Y strength (MPa)</td>
<td>3.79</td>
<td>3.61</td>
<td>3.67</td>
<td>3.86</td>
<td>3.75</td>
<td>3.80</td>
<td>3.94</td>
</tr>
<tr>
<td>Average (MPa)</td>
<td>3.40</td>
<td>3.40</td>
<td>3.51</td>
<td>3.56</td>
<td>3.50</td>
<td>3.59</td>
<td>3.67</td>
</tr>
<tr>
<td>Standard deviation (MPa)</td>
<td>0.55</td>
<td>0.30</td>
<td>0.23</td>
<td>0.42</td>
<td>0.36</td>
<td>0.30</td>
<td>0.37</td>
</tr>
</tbody>
</table>

Crack patterns of different sized meshes are shown in Figure 5-34. For meshes under 20 mm, different crack patterns were obtained. This was mainly because of the strong boundary effects. The macro-cracks distributed everywhere in the mesh, especially at locations where voids present. However, when the mesh sizes were greater than 20 mm, the macro-cracks appears to be concentrated to form dominant crack paths, due to the propagation of micro-cracks.

(a) 10×10 (ε=0.000286)  
(b) 15×15 (ε=0.000191)
Chapter 5 2D XCT-Image Based Modelling

Figure 5-34 Crack patterns for different meshes

5.10.2 Centred meshes without voids
To eliminate the voids effect, six more meshes were constructed based on cross-section 371 in the \(yz\) plane in Figure 5-1. No voids were included, and the same centre was maintained. Table 5-4 shows the volume fraction of each phase in different mesh sizes. The corresponding \(\sigma-\varepsilon\) curves are plotted in Figure 5-35. A fine convergence was obtained in terms of \(\sigma-\varepsilon\) behaviour, which also demonstrates that the 2D mesh size of 37.2mm was sufficiently large as a representative area. As for the trend of predicted tensile strength, meshes without voids have better alignment with predictions found in literature (i.e. the size effect law). Besides, according to the statistical analysis results in Section 5.8, the predicted strength varies for different micro-structures. Thus multiple micro-
structures are needed to study the size effect on the predicted tensile strength, which will be discussed in the next section.

Table 5-4 Volume fraction of each phase in different mesh sizes

<table>
<thead>
<tr>
<th>Volume Fraction (%)</th>
<th>Mesh size (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>10</td>
</tr>
<tr>
<td>Aggregate</td>
<td>62.77</td>
</tr>
<tr>
<td>Cement</td>
<td>37.23</td>
</tr>
</tbody>
</table>

Figure 5-35 The $\sigma$-$\varepsilon$ curves for different mesh sizes

5.10.3 Multiple meshes for each size

Based on cross-section 1 in Figure 5-5, the maximum numbers of realisations of 10mm, 20mm and 30mm meshes were 36, 9 and 4, which corresponds to 50%, 65% and 76% overlap areas. The average value and standard deviation of predicted tensile strengths and voids volume fractions for each mesh are depicted in Figure 5-36. A relative clear decreasing trend for average tensile strength and the standard deviation with increasing the mesh size was observed. The average voids volume fraction did not varying much. The mean $\sigma$-$\varepsilon$ curves of meshes are shown in Figure 5-37. Similar results were found as centred meshes: when the mesh size varies, the linear increasing stage of $\sigma$-$\varepsilon$ curve was identical; however
the softening stage was significantly different and the gradient gradually became stable.

Figure 5-36 The predicted average tensile strengths and voids volume fractions for different meshes

![Graph showing predicted tensile strengths and voids volume fractions for different meshes.](image)

Figure 5-37 Mean $\sigma$-$\varepsilon$ curves for 10mm, 20mm and 30mm meshes

![Graph showing mean stress-strain curves for different mesh sizes.](image)

Furthermore, in order to reduce the influence of larger voids on small meshes, meshes of 10mm, 20mm, 30mm and 37.2mm with voids volume fraction lower than 0.9%, were carefully constructed and simulated. The number of realisations for each size was 25, 22, 21 and 19 respectively. The predicted average tensile strengths along with mesh sizes are shown in Figure 5-38. It is clear that without the influence of larger voids, the expected size effect trend for tensile strength
was obtained when multiple meshes were used for each size. It also indicates that the realisations for each mesh size should be as much as possible to ensure a statistical representation.

Figure 5-38 The predicted average tensile strengths of 10mm, 20mm, 30mm and 37.2mm meshes

5.11 Typical uniaxial compression results

In this section, the 2D mesh in Figure 5-5 was extended from uniaxial tension to uniaxial compression. The same 2D FE mesh was used as that for the tension tests. For the ease of comparison with later 3D FE simulations, the relative realistic elastic moduli of aggregate and cement were changed to 51GPa and 13.6GPa from micro-indentation tests. Other material properties were maintained as in Table 5-1. The same simulation parameters were used.

Figure 5-39 shows the $\sigma$-$\varepsilon$ curves under uniaxial compression, both in the $X$ and $Y$ directions. Similar to the tensile tests, identical elastic responses at the initial stage were obtained for both directions. In addition, from Figure 5-39, the elastic modulus of concrete specimen was estimated as 22.2GPa and 23.1GPa for $X$ and $Y$ loading conditions, respectively, which is quite close to the homogenisation result of 24.1GPa. The $X$-compression condition led to a higher strength of 31.1MPa, which corresponds to a higher $Y$ tensile strength (see Figure 5-16).
Notably, the simulations reserved quite high residue stresses even after the sample failed, which was around 5MPa for $Y$-compression and 22MPa for $X$-compression. This is mainly because the damage under compression is not similar to the tensile condition, which has straightforward cracks breaking through the whole sample. High strength aggregates could still hold more loads even after the sample failed.

![Figure 5-39 The predicted $\sigma$-$\varepsilon$ curves under $X$ and $Y$ compressions](image)

The corresponding crack patterns at maximum load under $X$ and $Y$ compression are shown in Figure 5-40. Most micro-cracks for each condition propagated parallel to the loading direction with slight diversions due to the complicated micro-structure. The micro-cracks were distributed all over the mesh, rather than connected to form major macro-cracking paths as under tension. The inclined macro-cracks were in fact the result of a combination of micro-cracks at the meso-scale level, with some of them opening in tension and some of them inclined subject to shear.
5.12 Summary

In this chapter, 2D meso-scale FE models have been developed based on high-resolution XCT images to simulate crack propagation processes in concrete. The 2D images were first extracted from the segmented Brazilian-like image model described in Chapter 3. Following certain image processing procedures, the 2D images were transformed into FE meshes with the zigzagged boundaries smoothed. Then the zero-thickness cohesive interface elements with normal/shear traction–separation constitutive laws were embedded to simulate potential cracks in the cement and on aggregate-cement interfaces. Efficient codes were designed to process a large number of 2D images into FE meshes.

Simulations of uniaxial tension tests were conducted. The flexibility and effectiveness of the pre-inserting CIE technique in modelling realistic, complicated fracture processes is illustrated by the good qualitative and quantitative agreement of predicted results, experimental observations and other simulations. It is found that a large number of interfacial micro-cracks initiate very quickly and gradually become stable before the peak load is reached. Then the interfacial cracks continue to propagate and coalesce with newly formed cracks in the cement phase. The localised fracture shows that the cracking path is formed by bridging the initiated interfacial micro-cracks. In the meantime,
nearby cracks become unloaded and closed. The very different load-carrying capacities and crack patterns at different locations in the same specimen, demonstrate not only the effects of random distribution of phases, which can only be captured by the realistic meso-scale simulations, but also the limitations of 2D modelling and the necessity of 3D modelling. This study also shows that there exists a statistically inversely proportionated relationship between the predicted tensile strength and the void volume fraction, and the relative ratio of cohesive strength in the cement and on the aggregate-cement interfaces is a dominant factor in the micro-cracking behaviour, which in turn affects macro-cracking and the load-carrying capacities of the specimens. It can be concluded that the cracks always connect the shortest paths of the nearby interfacial elements that are perpendicular to the loading direction. Furthermore, parametric study results show the effects of the control parameters of the CIEs, initial stiffness and boundary conditions for the tensile tests.

The size effect study results show that the minimum size considered as a representative area for fracture modelling is four times the particle size for this concrete mixture, which in turn indicated that the model size of 37.2mm for 2D FE simulations was reasonable. The crack pattern remains almost constant when the model size increases above the representative area. The initial pre-peak behaviour of the stress-strain curve remains constant for different sizes and the predicted overall strength varies with a small deviation. More pronounced size effects can be found on the softening stage of the stress-strain curve. The conclusion can also be made that the voids (both the volume fraction and the size of larger voids) played an important role on size effect study.

Finally, the same 2D FE mesh used for the typical uniaxial tensile test in Section 5.3 was used to conduct compressive simulations. For the ease of comparison with 3D FE simulations in the next chapter, material properties were changed to the test values in Chapter 4. By comparing the 2D compressive simulations with the previous homogenisation estimation, very close values were obtained for the elastic modulus of the concrete specimen. It is found that this cross-section 1 in the xy plane has a higher compressive strength when the load was applied in the
$X$-direction than in the $Y$ direction. Very high residue stresses were found for both loading cases.
Chapter 6

3D XCT-Image Based Modelling

This chapter presents the 3D image based numerical simulation results. In Chapter 3, the in-situ XCT experiments were conducted and the scanned images were segmented. In Chapter 4, the elastic properties of the aggregate and the cement were measured by micro-indentation tests. This chapter extends the 2D image based modelling work presented in Chapter 5 to 3D. Both the 40mm cube under Brazilian-like compression and the 20mm cube (Sample 2) under uniaxial compression were simulated using the per-inserting cohesive interface element approach.

6.1 3D finite element mesh and material parameters

6.1.1 Generation of 3D finite element meshes

The 3D segmented concrete models built in Chapter 3 (Figures 3-13 and 3-32) were directly converted into 3D FE meshes using the commercial packages Simpleware (Simpleware, 2011) and AVIZO (AVIZO, 2013). The segmented images were exported from AVIZO and then imported into the ScanIP (Simpleware). Two different meshing algorithms are existed in ScanIP: FE grid and FE free. As the basic meshing module, the former builds tetrahedral or hexahedra (or sometimes mixed) meshes based on the voxels, which is fast and robust, however with less control on the mesh density and often resulting in very dense output meshes. In comparison, the latter is an advanced meshing module, which can only generate tetrahedral meshes. It has a greater flexibility in the elements creation process which allows more control over the number of elements than FE grid. However, the meshing process is often slower and time-
Chapter 6 3D XCT-Image Based Modelling

Consuming. In this research, FE free method was used. The advanced parameters of target minimum edge length and maximum edge length are 0.1mm and 0.5mm respectively. For the ease of segmentation, the 40mm cube concrete specimen was cropped into a 37.2mm cube and exported for FE mesh generation. This may cause potential problems (such as the size from the simulation is smaller than the test) when validating the 3D FE simulation. However, the uneven surfaces of the 40mm cube would unnecessarily increase the difficulties for image segmentation and cause stress concentrations during FE analyses. Furthermore, the uneven surfaces would need more complicated boundary conditions and thus have convergence problems during the nonlinear FE simulations.

Due to the difficulties involved to generate successful 3D FE meshes, the boundaries between the phases were smoothed before meshing. Table 6-1 summarises the Volume fraction alteration of the 40mm cube between the image model and the smoothed 3D mesh. 2.7% reduction and 3.9% increase were found in aggregates and cement respectively. However, before and after smoothing, the total number of elements for 40mm cube changes from 4,155,799 to 806,576 (around 80% reduction) when the same meshing parameters were used. The computational cost was too much for the 3D meshes without smoothing, even for computer clusters with 144 cores. Thus the compliance of volume fraction alteration was considered reasonable in this research.

<table>
<thead>
<tr>
<th></th>
<th>Aggregate $V_{F_a}$ (%)</th>
<th>Cement $V_{F_c}$ (%)</th>
<th>Voids $V_{F_v}$ (%)</th>
<th>Total volume (mm$^3$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Image model</td>
<td>49.6</td>
<td>49.7</td>
<td>0.7</td>
<td>51479</td>
</tr>
<tr>
<td>Smoothed 3D mesh</td>
<td>46.9</td>
<td>52.6</td>
<td>0.5</td>
<td>51479</td>
</tr>
</tbody>
</table>

The generated meshes were then exported into input files that are directly usable for FE analyses in ABAQUS (ABAQUS, 2010). Both the 40mm cube under the Brazilian-like test (cube size 37.2mm) and the 20mm cube under uniaxial

153
compression (Sample 2) were modelled. The aggregates and cement were treated as different element sets in the FE mesh. Voids were considered as empty areas. The converted 3D meshes are shown in Figure 6-1.

![Figure 6-1 3D FE meshes of the 40mm benchmark cube and the 20mm cube (Sample 2)](image)

A few smaller models cut from the 37.2mm full model were simulated first to test the viability and robustness of the explicit solver of ABAQUS in solving the complicated nonlinear problem with material softening caused by fracture. Two examples of 10mm (RVE10) and 20mm (RVE20) without CIEs inserted are given as examples are shown in Figure 6-2.

![Figure 6-2 3D FE meshes of RVE10 and RVE20 cut from 40mm cube](image)
6.1.2 3D CIE insertion

Similar to the 2D modelling, a 3D CIEs insertion procedure designed for homogeneous materials in (Yang et al., 2009; Su et al., 2010b) was extended to account for multiple phases and interfaces. The topology in 3D is more complicated and the cohesive elements are surfaces with zero thickness (rather than lines in 2D). Three sets of CIEs with different traction-separation laws were inserted all over the meshes, namely, CIE_AGG within the aggregate, CIE_CEM within the cement, and CIE_INT on the aggregate-cement interfaces.

The main 3D CIEs insertion code includes the following stages:

1. Import initial 3D mesh information, and sort out the nodal coordinates and the nodal connectivity of the solid elements;
2. Build the Node, Element and Face structures of the solid elements, which include index, topological connectivity and marks of each type according to the positions (e.g. mark the aggregate nodes with 1, cement nodes with 2, and interface nodes with 3);
3. Insert new nodes. For every single node (except those on the outer edges of the mesh), N numbers of new nodes were generated with the same coordinates when this node connects to N number of solid elements. The new nodes were stored in a new structure similar to the Node structure;
4. Update the topological structures of the solid elements in step 2;
5. Generate CIEs of three types. The CIEs are built by connecting the two faces (connecting new nodes generated in step 3) between the two neighbouring solid elements. Referring to the marks of the new nodes, three types of CIEs are distinguished by their positions (in aggregates, cement, or on interfaces);
6. Export new mesh information. There are two types of solid element sets named as aggregate and cement, and three types of CIE sets according to their positions. The nodes and element sets relating to the different phases were exported in the format of an ABAQUS input file.

Figure 6-3 shows the 10mm model with inserted CIEs (in red colour) surrounding the aggregate elements. The initial model has 30,766 nodes and
137,774 C3D4 tetrahedron solid elements, including 64,670 aggregate elements and 73,104 cement elements. After the insertion of CIEs, the total number of elements was increased to 379,716, with 241,942 cohesive elements (COH3D6) inserted. It is noteworthy that as the model gets bigger, more CIEs are inserted. This is a drawback of the model, as more nonlinear CIEs lead to much higher computational cost.

Figure 6-3 The CIEs (in red) surrounding aggregate elements in a 10mm cube model

6.1.3 Material parameters

The solid elements for aggregates and cement were assumed to behave linear elastically. The linear tension/shear softening laws were used to model CIEs, with the quadratic nominal stress initiation criterion, energy based damage evolution, and mixed-mode BK-law fracture energy criterion (ABAQUS, 2010). The material properties are shown in Table 6-2. The Young’s moduli of the aggregates and the cement were 51GPa and 13.6GPa from the micro-indentation tests in Chapter 4. The elastic stiffness in the shear directions ($k_s$ and $k_t$) was assumed to be the same as the normal direction ($k_n$). The cohesive strength in the shear ($t_s$ and $t_t$) was assumed as twice that of the normal direction ($t_n$). The power of 2 was used to define the BK-law fracture energy criterion. The fracture energy
in shear ($G_{Fy}$ and $G_{Fz}$) was assumed as 10 times the value in the normal direction ($G_{Fn}$) (López et al., 2008b).

A displacement-controlled loading scheme was used for all the simulations. The only difference between compression and tension is the loading direction. The ABAQUS/Explicit solver was used for the nonlinear equation systems with a step time of 0.01s. This was found to be sufficiently long to ensure a quasi-static loading condition. 32 cores in a computer cluster were used to tackle the much higher number of degrees of freedom of the FE meshes than 2D.

### 6.2 Modelling and validation of 40mm cube

The 37.2mm cube under the Brazilian-like compression was modelled with boundary conditions as close as those in the test (Figure 3-2b). The bottom loaded area was fully fixed in three directions ($x/y/z$) and the top loaded area was applied with a uniformly distributed displacement (Figure 6-4).

<table>
<thead>
<tr>
<th>Material</th>
<th>Young’s modulus $E$ (MPa)</th>
<th>Poisson’s ratio $\mu$</th>
<th>Density $\rho$ (kg/m$^3$)</th>
<th>Elastic stiffness $k_n$ (MPa/mm)</th>
<th>Cohesive strength $t_n$ (MPa)</th>
<th>Fracture energy $G_{Fn}$ (N/mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aggregate</td>
<td>51000</td>
<td>0.2</td>
<td>2500</td>
<td>/</td>
<td>/</td>
<td>/</td>
</tr>
<tr>
<td>Cement</td>
<td>13600</td>
<td>0.2</td>
<td>2200</td>
<td>/</td>
<td>/</td>
<td>/</td>
</tr>
<tr>
<td>CIE_AGG</td>
<td>/</td>
<td>/</td>
<td>2500</td>
<td>$10^6$</td>
<td>/</td>
<td>/</td>
</tr>
<tr>
<td>CIE_CEM</td>
<td>/</td>
<td>/</td>
<td>2200</td>
<td>$10^6$</td>
<td>6</td>
<td>0.06</td>
</tr>
<tr>
<td>CIE_INT</td>
<td>/</td>
<td>/</td>
<td>2200</td>
<td>$10^6$</td>
<td>3</td>
<td>0.03</td>
</tr>
</tbody>
</table>
Figure 6-4 Boundary conditions of the 40mm cube under the Brazilian-like compression

6.2.1 Force-displacement curves

The DVC modified force-displacement \((F-d)\) curve of the in-situ Brazilian-like compression test (Figure 3-5) and the 3D FE simulation result are shown in Figure 6-5. The predicted peak load 16.3kN from the simulation is close to the experimental value 16.5kN. The post-peak softening stage that cannot be obtained by the test was well captured. However, a too soft initial stage was obtained. Besides some unknown uncertainties involved in the XCT test, one main reason may be that the displacement calculated from the DVC technique was averaged on the whole cross-section of 37.2mm\(^2\), rather than the loading area of 17.5mm\(^2\) as in the FE simulation.

![Figure 6-5 Comparison of F-d curves from DVC and the 3D FE simulation](image)
6.2.2 Crack patterns

The crack pattern of the in-situ specimen has been reconstructed using AVIZO software, and the comparison with the simulated one is shown in Figure 6-6 and Figure 6-7. Simulation provides a good agreement with the experiment in terms of overall crack path, at both the peak load and the post-peak stage. In this Chapter, the CIEs with the damage index SDEG\textgeq0.99 are regarded as macro-cracks.

**Peak load**

The surface crack pattern at the peak load from the XCT test (Figure 6-6a) looks quite similar to that from the simulation shown in Figure 6-6b. Figure 6-6c and Figure 6-6d show the internal cracks from the XCT scan and the simulation. It looks that most of the inner micro-cracks were predicted. The similarity of crack patterns both on the surface and in the interior indicates the capability of the proposed image-based modelling technique in predicting 3D crack propagation in concrete.
Post-peak stage

The crack patterns on a few slices from the XCT test (post scan at 13.5kN) and the FE simulations inside the concrete specimen are shown in Figure 6-7, in which a, c and e are the XCT images, and b, d, and f are the simulated results. A reasonable resemblance in the crack pattern can be noticed. The complicated crack patterns are reflections of the randomly distributed multi-phases. The difference between the test and the simulation may be caused by smoothing of aggregates, which was used to simplify the FE meshes for better numerical stability.
6.2.3 Internal crack propagation

Figure 6-8 shows the damage evolution in CIEs in the cement and on the interfaces as the displacement progresses. At an early stage with \(d=0.0067\)mm (Figure 6-8a), many interfacial cohesive elements started to damage, mainly concentrated in the central volume between the loading rigs. The cracks propagated quickly until these CIEs fully failed. Once the damage penetrated the cube in the loading direction (Z), cracks started to expand in the horizontal directions (X and Y). Finally, the model failed when the interfacial cracks were connected by the cracks in the cement. The ability of the simulations to unveil the damage and fracture evolution in any number of loading steps is a
considerable advantage over in-situ XCT tests, because these tests are still very expensive and usually a few scans at selected load levels can be conducted, subjected to budget and time limits.

Figure 6-8 Damage evolution in the cement and on the interfaces
Figure 6-9 shows the fully damaged elements with $\textit{SDEG}$ over 0.99. It can be clearly seen that the failed elements first existed near loading surfaces, and then propagated in the loading direction ($Z$). Once the cracks coalesced in the $Z$ direction, the damage started to expand in the horizontal directions ($X$ and $Y$). The red coloured areas represent the fully damaged macro-cracks.

Figure 6-9 Damage propagation with $\textit{SDEG}$ over 0.99 ($\textit{DSF}$=10)
6.3 Modelling and validation of 20mm cube

The 20mm cube under uniaxial compression test was then modelled, and the results were compared with the in-situ XCT test data.

6.3.1 Force-displacement curves
Figure 6-10 shows the $F-d$ curves from the experiment (corrected by DVC in Figure 3-17) and the FE simulation. The two curves are quite similar before the peak load, which is 9.1kN and 9.5kN for the XCT test and the simulation, respectively. In addition, the slope of the linear section of the test up to 3kN, namely, the elastic modulus of the cube, is 23.6GPa, which is slightly higher than the modelled 20.6GPa.

![Force-displacement curves](image)

Figure 6-10 $F-d$ curves of 20mm Sample 2 from test and FE simulation

6.3.2 Crack propagation
Figure 6-11 compares the crack propagation processes at different loadings from the 3D simulation and the in-situ XCT images. Figure 6-11a shows the segmented image with initial microcracks and voids, and Figure 6-11b shows the FE model simulating the voids only without loading. It can be noticed that most of the voids (including the missing corner) were characterised in the FE model. The initial microcracks are not modelled because they were disappeared when
smoothing and meshing the image model due to their small volumes in 3D. In addition, these small 3D volumes with small FE elements will often cause numerical problems. Figure 6-11c and Figure 6-11d highlight the newly propagated or generated cracks at 5kN. From both the experiment and FE simulation, a small number of cracks can be seen, with most of them distributed in the central part of the cube. The crack patterns at the peak load are shown in Figure 6-11e and Figure 6-11f, respectively. They look different. Several reasons were involved. The primary one is that the boundary condition in the test was complicated, and the compressive load was not applied purely uniaxial as in the FE simulations. Besides, the top and bottom surfaces of sample 2 in the experiment were not perfectly parallel, which will cause force concentration on specific areas and thus generate concentrated cracking areas like Figure 6-11e. For the FE simulation, the mesh was cropped into an ideal cube when reconstructing. Furthermore, the uniaxial load was easily applied on the parallel surfaces. A more accurate FE mesh and realistic boundary conditions should help to generate more realistic damage patterns, as in the in-situ experiment. Compromises have to be made to conduct 3D FE simulation, but the overall $F-d$ curve as well as pre-peak crack pattern agrees well.

(a) XCT-0kN  
(b) FE simulation without load
Figure 6-11 Comparison of damage propagation characterised from the in-situ XCT tomography images and the FE simulation

Following the different cracks propagated at peak load, different final crack patterns occurred which are shown in Figure 6-12. However, the common phenomenon is that the cracks always propagated through or near defects, with most of them parallel to the compressive loading direction. The macro-cracks might be diverted at some local areas due to the complex distribution of phases.
6.4 Uniaxial compression test of 40mm cube

For the 40mm benchmark cube, uniaxial compression simulations were also conducted. After elastic simulation of the benchmark cube, the elastic modulus of the concrete cube was estimated and compared by different techniques. Furthermore, the volume size effect on the $\sigma$-$\varepsilon$ curve of benchmark cube was also investigated. The detailed results are presented in the following sections.

6.4.1 Elastic simulation

The elastic modelling of the uniaxial compression was conducted prior to the insertion of CIEs. Only elastic modulus and Poisson’ ratio in Table 6-2 were assigned to the aggregate and the cement elements. The ABAQUS/general static solver was used. The bottom surfaces were fully fixed ($x=y=z=0$) and the top surfaces were applied with distributed forces. Figure 6-13 shows the simulated stress distribution in the $Z$ direction ($S_{33}$) in the concrete, for both the benchmark cube and sample 2. It can be seen that the high compressive stresses were mostly encountered in the aggregates as expected, due to their higher elastic modulus. Less compaction was found in the cement. Some cement areas between aggregates that are parallel to the loading direction even appeared to have high tension forces. Besides, these tensile forces seem to be connected in sample 2.
with the smaller cube size and are distributed in the larger benchmark cube. Furthermore, the identical $F-d$ curves for the elastic modelling of the benchmark cube and sample 2 can be used to validate the elastic stage of the fracture modelling results under the same boundary conditions.

![Figure 6-13 Stress distribution in the Z direction (S_{33})](image)

6.4.2 Fracture modelling of the 40mm cube

Fracture modelling of uniaxial compression was then simulated using the same benchmark cube and material properties in Table 6-2. Instead of being limited to a concentrated area, the load and restriction areas were applied on the whole top and bottom surfaces. Figure 6-14 shows the stress-strain ($\sigma$-$\varepsilon$) curves of the elastic and fracture modelling simulations, as well as the 2D uniaxial compression in Chapter 5.11.
From Figure 6-14, it can be seen that all the simulations match well at the initial elastic stage. Then, unlike the elastic simulation, the fracture modelling curves of the 2D and 3D simulations started to enter into the hardening stage and gradually reached the peak load. Higher compressive strength and larger final strain were obtained in the 3D simulation than in the 2D. In comparison with the 2D $\sigma$-$\varepsilon$ curve, the prolonged hardening and softening stages of 3D modelling suggest that 3D fracture behaviour is far more complicated and greatly depends on the inhomogeneous 3D distributions of each phase in the concrete. This can be confirmed by the comparison of crack patterns in 3D and 2D, which are shown in Figure 6-15. It is obvious that cracking in concrete is related to all the three dimensions. This is why it is necessary to conduct fracture modelling in 3D. Furthermore, from Figure 6-16, one can see that the internal damage at the peak load was already developed and distributed all over, which is quite different to the Brazilian-like loading case.
6.4.3 Effective elastic modulus validation

The Young’s modulus ($E$) of the benchmark concrete cube under uniaxial compression was validated by comparing estimations from bounding methods (lower and upper bounds), homogenisation, 2D fracture simulation, 3D elastic simulation and 3D fracture modelling. This is illustrated in Table 6-3. Similar results were obtained by different techniques. This in turn also validated the accuracy of the elastic stage of the 3D fracture modelling simulation under uniaxial compression.
Table 6-3 Comparison of estimated Young’s modulus by different techniques

<table>
<thead>
<tr>
<th>Technique</th>
<th>Boundin g methods</th>
<th>Homogeneity</th>
<th>2D fracture simulation</th>
<th>3D elastic simulation</th>
<th>3D fracture modelling</th>
</tr>
</thead>
<tbody>
<tr>
<td>Estimation of $E$ (GPa)</td>
<td>22-34</td>
<td>24.16</td>
<td>23.1</td>
<td>25.8</td>
<td>24.3</td>
</tr>
</tbody>
</table>

6.4.4 Volume size effect

To study the volume size effect on fracture test under uniaxial compression, different realisations were cropped for 10mm (RVE10) and 20mm (RVE20) cubes from the benchmark cube. There are 5 realisations in total for RVE10, and 3 for RVE20. The numbers after RVE10 and RVE20 represent the corresponding realisations; e.g. RVE10_1 means the first realisation of RVE10. The material properties in Table 6-2 were used.

The volumetric average $\sigma$-$\varepsilon$ curves for 5 realisations of RVE10, 3 realisations of RVE20 and the full model loaded under $X/Y/Z$ are shown in Figure 6-17. Similar to the 2D size effect studies, identical initial elastic responses were obtained. There is no evident size effect on the compressive strength. The influence of volume size is mainly on the softening stage. With increasing cube size, the brittleness of the sample increases and the final strain reduces.

Figure 6-17 volumetric average $\sigma$-$\varepsilon$ curves of different volume sizes under compression
The uncertainties involved in different realisations for each volume size are illustrated by the figures from Figure 6-18 to Figure 6-20. For each volume size, there exist few differences both on the compressive strength and the softening stage. The elastic stage was identical though. For different load directions of benchmark cube, consistent results were obtained.

**Figure 6-18** $\sigma$-$\varepsilon$ curves for realisations of RVE10

**Figure 6-19** $\sigma$-$\varepsilon$ curves for realisations of RVE20

**Figure 6-20** $\sigma$-$\varepsilon$ curves for benchmark cube under $X/Y/Z$ loads

172
6.5 Uniaxial tension test

Uniaxial tension tests were simulated for the 20mm cube (sample 2), and the 40mm benchmark cube. Material properties in Table 5-1, which were used in references (Caballero et al., 2005; López et al., 2008a) and the 2D image based modelling under tension in Chapter 5, were used here for 3D tensile simulations. For all the uniaxial tensile tests, the bottom surfaces were fully constrained and the top surfaces were applied with displacement controlled forces. The ABAQUS/ Explicit solver was used.

6.5.1 20mm cube (sample 2)

For the uniaxial tensile tests, sample 2 was first used to compare with the results from reference (Caballero et al., 2005). Figure 6-21 shows the $\sigma$-$\varepsilon$ curves. It can be seen that identical initial elastic stages, and broadly similar overall behaviour, was obtained. The differences of peak loads and softening responses were mainly due to variances of sample size and phase proportions.

![Figure 6-21 $\sigma$-$\varepsilon$ curves under uniaxial tension (volume fractions of aggregates are 54.8% and 20% for the present sample 2 and the reference (Caballero et al., 2005), respectively)](image)

The micro-crack initiation, and evolution at different loading stages (loading points of A, B, C and D in Figure 6-21), are shown in Figure 6-22. The cohesive
elements in red represent micro-cracks. Before point A, there were few damaged elements in the cube. However many micro-cracks initiated very quickly before reaching the peak load (C). At peak point C, the micro-cracks already became very complicated and had propagated.

![Figure 6-22 The initiation and propagation of micro-cracks](image)

The final macro-crack pattern is shown in Figure 6-23. It can be seen that, unlike complicated micro-crack distribution in Figure 6-22, the 3D crack path was
finally formed by connecting interfacial cracks and those in the cement. The specimen was split into two pieces. Besides, the internal 3D crack surfaces confirm that the internal cracking is a very complicated process, and this in turn proves that 3D FE simulation is a very powerful tool.

Figure 6-23 Final macro-crack pattern of sample 2 under tension

6.5.2 10mm RVE10_1 of benchmark cube

Prior to simulate the full-model of the benchmark cube, a smaller volume of RVE10_1 was used to conduct a uniaxial tensile test. The typical tensile behaviour in concrete was illustrated in detail. The corresponding $\sigma$-$\epsilon$ curve is shown in Figure 6-24.
Figure 6-24 shows the process of initiation and coalescence of micro-cracks and macro-cracks (corresponding to the points marked A, B, C, D and E in Figure 6-24). The blue areas represent aggregates. The orange and red (darker) colours represent the micro-cracks, which exist on the aggregate-cement interfaces and within the cement. Many micro-cracks initiated on the aggregate-cement interfaces at Point A. At point B, more micro-cracks appeared. Some of them begin to coalesce, and connected by newly formed micro-cracks in the cement. Most of interfacial micro-cracks formed before the peak load (at point C). Meanwhile, more and more micro-cracks mainly occurred in the cement (at point D) and the micro-cracks are gradually developed into macro-cracks. Finally the specimen split into two pieces (at point E). The cracked specimen is shown in Figure 6-25f. This complex cracking process in Figure 6-25 shows that the interfacial micro-cracks were firstly occurred and gradually became stable until the peak strength was reached. Then the micro-cracks in cement became dominant during post-peak stage and finally cracked the sample.
Chapter 6 3D XCT-Image Based Modelling

(a) A (\(\varepsilon = 0.00017\))  
(b) B (\(\varepsilon = 0.00029\))  
(c) C (peak, \(\varepsilon = 0.00044\))  
(d) D (\(\varepsilon = 0.00086\))  
(e) E (\(\varepsilon = 0.00375\))  
(f) Final macro-crack

Figure 6-25 The initiation and propagation of micro- and macro-cracks

The final cracked surfaces are shown in Figure 6-26. The numbers (\(\textcircled{1}-\textcircled{5}\)) represent five aggregates (in blue colour) around the cracked surface. As no cracks are allowed through aggregates, the crack surfaces always formed around aggregates. The numbers (\(\textcircled{1}-\textcircled{5}\)) in Figure 6-26b are the corresponding places in Figure 6-26a, which caused the resulting crack path.
6.5.3 40mm benchmark cube

Finally, the 40mm cube was used to conduct full-model fracture modelling under uniaxial tension. The comparison of $\sigma$-$\varepsilon$ curves in 3D and the mean curve of 2D slices in Figure 5-22, shows that the cube in 3D has a higher tensile strength (5.0MPa) than in 2D (3.3MPa). One reason may be that the formation of cracks in the 3D sample is more difficult, due to the obstruction from arbitrary distributed phases with quite different shapes (Yin et al., 2013). Another one could be the larger fracture surfaces in 3D, which provides higher normal traction (Su et al., 2010b).

![Figure 6-26 Final cracked surfaces of RVE10](image)

![Figure 6-27 $\sigma$-$\varepsilon$ curve in 3D and 2D mean](image)
The 3D final crack pattern is shown in Figure 6-28. Similar to previous uniaxial tension simulations, a full crack path was formed at last, with complex surfaces diverted by the heterogeneous distribution of phases (i.e. aggregates and voids) in the sample.

![Figure 6-28 Final crack pattern (DSF=10)](image)

The internal 3D crack surfaces at peak load and the final step are shown in Figure 6-29. The distributed 3D crack surfaces at peak load in Figure 6-29a indicate that there is still no dominant crack path at this stage. As the increase of external load (Figure 6-29 b and c), some of the distributed micro-cracks are gradually connected and some of them are closed. Finally, the 3D crack surfaces (Figure 6-29d) were connected to form the major macro-crack path.

![Figure 6-29 Distributed 3D crack surfaces at peak load and the final step](image)

(a) peak load (DSF=50)  (b) Post-peak-1 (DSF=20)
6.5.4 Volume size effect

Similar to the volume size effect under uniaxial compression in Section 6.4.4, the realisations of RVE10 and RVE20, as well as the full-model of the 40mm cube were modelled to conduct volume size effect study under uniaxial tension.

Figure 6-30 shows the averaged $\sigma$-$\varepsilon$ curves for 5 realisations of RVE10, 3 realisations of RVE20 and the full model loaded under $X/Y/Z$. Again, very close initial elastic responses were obtained. A small size effect on the averaged tensile strength was found, i.e. 5.05MPa for RVE10, 4.95MPa for RVE20 and 4.87MPa for the full-model. However, the softening stages varied greatly. The brittleness increases with increasing cube volume size.
The $\sigma$-$\varepsilon$ curves for 5 realisations of RVE10 in Figure 6-31 and 3 realisations of RVE 20 in Figure 6-32 indicate that little variation was found for different realisations of different volume sizes, both on the peak strength and the post-peak softening stage. However, Figure 6-33 plots quite different $\sigma$-$\varepsilon$ curves for the full-model loaded under X/Y/Z. Unlike similar $\sigma$-$\varepsilon$ curves under uniaxial compression, the simulations under tension predict different behaviours, which contribute from the heterogeneous distribution of phases. Especially for Y-load, it showed a lower tensile strength of 4.54MPa (around 10% less than 5.02MPa and 5.04MPa for X-load and Z-load). This is attributes to the arrangement of the two big voids in the middle of the model: they were laid along the Y direction (see Figure 3-9) and provided potential weak links. The elastic behaviour before peak strength for each sized volume maintained identical though.

![Figure 6-31 $\sigma$-$\varepsilon$ curves for realisations of RVE10](image1)

![Figure 6-32 $\sigma$-$\varepsilon$ curves for realisations of RVE20](image2)
Chapter 6 3D XCT-Image Based Modelling

6.6 Summary

The 3D FE meshes of the 40mm benchmark cube and the 20mm Sample 2 were constructed based on the segmented image models in Chapter 3. FE meshes with smaller volumes from the 40mm cube were also constructed to investigate the volume size effect. The 2D CIE insertion program was extended into 3D to represent the potential cracks. The Young’s moduli of the aggregates and the cement obtained from the micro-indentation experiments were used in the FE simulations.

3D FE simulations were conducted for both the Brazilian-like compression test of benchmark cube and the uniaxial compression test of Sample 2. The simulated $F-d$ curves and the crack propagation were validated by in-situ XCT results. There are many reasons why the 3D fracture modelling results do not perfectly match the in-situ XCT experiment. The first one would be the compromises made when generating the 3D meshes, such as smoothing of phases during image segmentation and FE mesh transformation. Because cracking in concrete is a highly localised behaviour, it relies greatly on the distribution of different phases. The compromises would potentially alter the crack path in certain circumstances. Another main reason is that the boundary conditions (both loading and displacement restrictions) in the experiments are far more complicated than in

Figure 6-33 $\sigma$-$\varepsilon$ curves for benchmark cube under $X/Y/Z$ loads
the FE modelling. FE simulations can use perfect boundary conditions, such as paralleled surfaces and ideally positioned forces. However, more detailed and continuous crack propagation processes can be obtained from FE simulations. Also, it is easy to apply complicated loading conditions, which are often difficult in real tests.

Furthermore, a uniaxial compression test was conducted for the benchmark cube. The elastic modulus was validated by different techniques used in this research. The volume size effect study indicates that the brittleness of the sample increases with increases in the cube size. The opposite trend was found on the final strain. Finally, uniaxial tensile simulations confirmed the flexibility and effectiveness of the developed image based modelling technique.
Chapter 7

Concluding Remarks and Future Work

This chapter presents the concluding remarks from the XCT image based fracture modelling. Several key aspects and findings are illustrated from the in-situ experiment, and the 2D and 3D FE simulations. Finally, some recommendations for future work are made.

7.1 Schematic of the proposed technique

As illustrated in Chapter 1, this research targets developing a schematic of in-situ XCT characterisation and meso-scale image based fracture modelling of concrete. Following the studies from Chapter 2 to 6, a flowchart of the proposed technique is given in Figure 7-1.

Figure 7-1 Modelling scheme
More specifically, after the concrete mixture (potentially any material) was prepared, the in-situ XCT scans were conducted at continuous loading steps. Then the 3D image models with realistic internal micro-structures were reconstructed and segmented. Before FE transformation, resample and surface simplification operations were conducted to ensure the generation of successful and usable meshes. Then 2D or 3D FE meshes were constructed. Further simplifications were made if the mesh was too dense or not successful. The CIEs were then embedded in the meshes to represent potential cracks. Finally, the in-situ scanned images were used to validate the FE simulation results.

### 7.2 In-situ experiments

Based on the fact that different components of a material have different abilities to attenuate X-ray beams, XCT has been widely used for medical imaging as well as engineering applications. In this research, concrete cubes were cast in the laboratory and a Brazilian-like compression test was conducted as a benchmark test, as well as further uniaxial and cyclic compression tests.

As a benchmark test, the 40mm cube was loaded and in-situ scanned at different loading steps. A realistic cube was reconstructed virtually and segmented to distinguish different phases, namely, aggregate, cement and voids. However, manual operations were involved during segmentation, due to the low contrast between aggregate and cement. Thus, more automatic and efficient algorithms need to be developed in the future.

Two more 20mm cubes with the same mixture, were cropped and used to conduct in-situ XCT scans for monotonic compression and cyclic compression tests. The fracture features were characterised and illustrated in detailed through both 2D tomography images and 3D sub-volumes. Moreover, the 3D distribution of voids and cracks unveiled the crack propagation in 3D. Crack transition zones and interfacial transition zones were proposed, and measured through XCT images. The average measurement of the ITZ thickness is $0.157 \pm 0.028\,\text{mm}$. The equivalent diameter of aggregate measured from sample 2 is $3.88 \pm 1.24\,\text{mm}$. 
However for voids, the measured equivalent diameter is $0.72 \pm 0.62 \text{mm}$. All the statistical information in this deterministic concrete specimen could be used for generating many random concrete models. The segmented 3D image models supported a reliable micro-structure for 2D and 3D image based FE simulations.

Furthermore, material properties of the concrete cube were tested and estimated by micro-indentation and homogenisation techniques. The average value of Young’s modulus of aggregate and cement were 51GPa and 13.6GPa respectively. These values were used for 3D FE fracture simulations. The estimated effective homogenised elastic modulus of concrete was 24.16GPa by homogenisation analysis.

### 7.3 2D investigation results

Two dimensional meso-scale image based FE models were developed to conduct fracture modelling simulations. 2D slice images of the Brazilian-like cube were first extracted and then transformed into FE meshes, with zigzagged boundaries been processed. Efficient programs were coded to process serial 2D images into FE meshes. With the help of embedding cohesive interface elements in the meshes, sufficient FE fracture simulations were conducted under uniaxial tension and compression.

From a large number of uniaxial tensile simulations, it was found that interfacial micro-cracks initiate quickly and gradually become stable before the peak load is reached. Then the interfacial cracks continue to propagate and coalesce with newly formed cracks in the cement phase. The specimen finally failed with dominant macro-cracks. The different load-carrying capacities and crack patterns at different locations in the same specimen demonstrate not only the effects of random distribution of phases which can only be captured by realistic meso-scale simulations, but also the limitations of 2D modelling, and thus the necessity of 3D modelling. This study shows that there exists a statistically inversely proportional relationship between the predicted tensile strength and the void volume fraction. It also shows that the relative ratio of cohesive strength in the
cement and at the aggregate-cement interfaces is a dominant factor in the micro-cracking behaviour, which in turn affects macro-cracking and the load-carrying capacities of specimens.

It is shown by the size effect study that the model size of 37.2mm for 2D fracture simulation is reasonably large to provide a representative area. The minimum representative area for this mixture is four times the averaged aggregate size. The initial pre-peak behaviour of the stress-strain curve remains constant for different sizes and the predicted overall strength varies with a small deviation.

Uniaxial compression simulations on the same 2D mesh indicate that the model has a higher compressive strength for X loading than for Y loading. High residue stresses were found for both loading conditions. Then the simulated force-displacement curve was used for comparison with the 3D simulation.

7.4 3D investigation results

Following the 2D model, a 3D meso-scale image based FE model technique was developed. After building the FE meshes and inserting the CIEs in 3D, fracture simulations of the Brazilian-like cube and the uniaxial compression cube of sample 2 were validated using experimental curves and tomography images. In terms of force-displacement curves, the simulated peak values are almost identical to the experiments. However, the FE simulations seem to underestimate the initial elastic properties. As for crack patterns, although differences were encountered, a good resemblance of the macro-crack path as well as internal cracking was obtained at both pre-peak and peak loads.

There are many reasons why the 3D fracture modelling results do not match perfectly with the in-situ XCT experiments. The first being the compromises made when generating the 3D mesh, such as smoothing the phases in concrete during image segmentation and FE mesh transformation. Cracking in concrete is a highly localised behaviour and relies greatly on the distribution of different phases. The compromises would potentially alter the crack path in certain
Chapter 7 Concluding Remarks and Future Work

circumstances. Another significant reason is that the boundary conditions both loading and restricting in the experiments are far more complicated. However, FE simulations could use perfect boundaries conditions, such as paralleled surfaces and ideal positioned force. Besides, more detailed and continuous crack propagation process can only be obtained from FE simulations. Also it is easy to apply complicated loading conditions, which are normally difficult to replicate in real tests.

A uniaxial compression test was conducted for the benchmark cube. The elastic modulus of the concrete cube was validated using different techniques (bounding methods, homogenisation, 2D fracture simulation, 3D elastic simulation and 3D fracture modelling). The $\sigma$-$\varepsilon$ curve of the fracture modelling in 3D showed prolonged hardening and softening stages, which suggests that 3D fracture behaviour is far more complicated and greatly depends on the inhomogeneous 3D distribution of each phase in concrete. The volume size effect study indicates that the influence of RVE size is mainly on the softening stage. With increases of cube size, the brittleness of the sample increases and the final strain reduces.

Finally, uniaxial tensile simulations were conducted. The comparison of sample 2 and a reference test in literature showed that a broad similarity was obtained. The detailed illustration of crack initiation and propagation, showing cracking on the aggregate-cement interfaces and in the cement, confirmed the flexibility and effectiveness of the proposed image based modelling technique.

In conclusion, the proposed approach of analysis of concrete fracture behaviour is a meaningful practice. It covers many issues relating to the fracture mechanism of concrete. However, it also has some problems and limitations, which require further development.

7.5 Future work

Following this research, several future items of work are suggested.
The 40mm specimen size of Brazilian-like test was selected due to the load-carrying capacity of the DEBEN loading system. As the development of the experimental techniques, larger specimen sizes could be used to investigate the representative feature and the size effect in concrete. The internal fracture features of different sizes could be visualised and compared. Moreover, multiple specimens for each size could be used to study the variability and to collect the statistical distribution of the uncertainties in concrete.

In order to build realistic FE meshes, high resolution images obtained from in-situ tests are usually required to be segmented. However, commercial software packages and manual interactions were involved in this research for all the scans, due to the low contrast between the aggregates and cement. Thus, improvements can be made both on enhancing the image contrasts between phases during scan (e.g. phase contrast XCT scan) and developing new codes to automatically process serial datasets. In addition, more in-situ XCT tests of practical concrete specimens, such as regular/ lightweight/ high-strength concrete can be potentially conducted using the proposed framework, and the loading conditions can be more sophisticated (e.g. biaxial/ dynamic loading).

The key stage of the proposed simulation technique is generating usable 3D FE meshes. Similar to the 2D meshing codes, efficient 3D codes need to be developed to optimise the mesh quality and improve the transforming efficiency without losing accuracy. The influences of smoothing and other simplification processes during meshing need to be evaluated. Parallel algorithms could be used to speed up both the mesh transformation and FE simulation times.

For the conducted fracture simulations in this thesis, the aggregates were assumed as elastic material. However, the cracking in aggregates (e.g. lightweight concrete) can also be simulated by assigning damage parameters to the cohesive elements inside of aggregates (CIE_AGG). Furthermore, more complicated loading conditions, such as biaxial loading, can also be conducted on the established 3D meshes. Following the proposed technique, the 3D FE
mesh of 20mm sample 4 can also be simulated and compared with the in-situ scanned images.

(5) Based on the scanned images of both the 40mm and 20mm cubes, smaller volumes with initial micro-cracks could be meshed and simulated at micro-scale. The effect of these initial defects on the fracture behaviour of concrete can be evaluated. What’s more, the simulation of interfacial behaviour and grain movements can also be conducted by constructing and simulating small volumes.

(6) To construct random concrete models based on the statistic information, such as 3D distribution of aggregates and voids, and to investigate the effectiveness and efficiency of the two methods. And ultimately, to propose multi-scale modelling techniques to upscale the image-based models to the full-sized structures so that the structural reliability can be assessed.
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196


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