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Microstructure-informed modelling of damage evolution in cement paste

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HIGHLIGHTS

- Macroscopic behaviour from microstructure features and meso-scale principles.
- Derivation of microstructure features from high-resolution micro-CT images.
- Construction of site-bond model with microstructure information.
- Demonstration of agreement between calculated responses and experimental data.
- Quantitative assessment of microstructure effects on macroscopic behaviour.

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ABSTRACT

Cement paste is a binder for cementitious materials and plays a critical role in their engineering-scale properties. Understanding fracture processes in such materials requires knowledge of damage evolution in cement paste. A site-bond model with elastic-brittle spring bundles is developed here for analysis of the mechanical behaviour of cement paste. It incorporates key microstructure information obtained from high resolution micro-CT. Volume fraction and size distribution of anhydrous cement grains are used for calculating model length scale and elasticity. Porosity and pore size distribution are used to allocate local failure energies. Macroscopic damage emerges from the generation of micro-crack population represented by bond removals. Effects of spatial distribution, porosity and sizes of pores on tensile strength and damage are investigated quantitatively. Results show a good agreement with experiment data, demonstrating that the proposed technology can predict mechanical and fracture behaviour of cementitious materials based exclusively on microstructure information.

1. Introduction

Concrete is the most popular and widely used construction material in the world. The fracture behaviour of concrete has been a great concern for many years and remains a challenge due to concrete's complex and heterogeneous porous microstructure extending over wide range of length scales from nanometres to millimetres [1]. At meso-scale, concrete can be considered as a three-phase composite consisting of aggregate, matrix (i.e. cement paste) and interfacial transition zone (ITZ) between aggregate and matrix. ITZ is a "special" cement paste that has a higher initial water-to-cement mass ratio (w/c) compared to matrix [2]. Therefore, to study the mechanical properties and failure of concrete, one must first understand the damage evolution and fracture process in cement paste, which depends on its microstructure.

In order to characterise the 3D microstructure of cement paste, a variety of techniques including computer-aided simulation and experimental tests have been proposed and developed in the past few decades. Among them, computer-based cement hydration models, e.g. CEMHYD3D [3], HYMOSTRUC3D [4,5] and the more recently proposed µic (pronounced Mike) [6] are commonly applied to simulate the hydration process and gradual formation of the microstructure of cement paste. As a non-destructive technique, X-ray micro-computed tomography (micro-CT) has many advantages compared to other experimental techniques and has been successfully utilised to obtain the 3D microstructure of cement paste at a high resolution of 0.5 µm/voxel [7].

Many approaches have been proposed to develop the so-call micromechanical models by taking into account the underlying microstructure and mechanical properties of components of cement paste in recent years [8–20]. The important feature of the micromechanical models is that the material damage at the continuous level is introduced by the nucleation and evolution of micro-

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cracks. Discrete lattice models that represent a material by a lattice system of beam or spring elements are the most popular micromechanical models and seem to offer promising modelling strategy to explain fracture processes in cement paste [20]. Based on the simplest regular lattice with cubic cells, a lattice beam model has been proposed by Schlangen and van Mier [8], and further developed and adopted by Qian [19] to simulate the fracture processes in cementitious materials at different length scales. However, it has been pointed out that this lattice is not physically realistic in terms of shape of the represented phases in cement paste and is unable to provide a linear elastic response with an appropriate elastic modulus and Poisson's ratio [21]. Moreover, the obtained stress–strain curves of cement paste under uniaxial tests remain not realistic [14]. Man [15] developed two more complex 3D lattice beam models based on face-centred cubic packing (fcc) and hexagonal close packing (hcp) to investigate the fracture behaviour of concrete at meso-scale. However, the effects of spatial and size distribution of pores were not taken into account.

To overcome such limitations a site-bond model using a bi-regular lattice of truncated octahedral cells for elasticity has been recently proposed by Jivkov and Yates [21] and subsequently used to simulate the micro-crack population and damage evolution in concrete accounting for pore size distribution [20,22,23]. The microstructure of concrete was represented by truncated octahedral cells, which were regarded as the best choice for a regular representation of a solid. The interactions between unit cells were modelled by structural beam elements. One problem of this model is that the relationship between the global elasticity and local element properties cannot be established analytically. To deal with this issue, the site-bond model for elasticity was reformulated by Zhang et al. [24] by using elastic springs instead of beams to represent the microscopic interactions between sites. The relationship between spring constants and macroscopic elastic parameters was analytically derived and validated.

The main purpose of this work is to develop the site-bond technology to study the macroscopic behaviour and damage evolution of cement paste considering its underlying microstructure attributes such as porosity, pore size distribution, volume fraction and particle size distribution of unhydrated cement. X-ray micro-CT along with image processing and analysis techniques is used to capture the microstructure features of cement paste. A site-bond assembly with sites at centres of truncated octahedral cells and bonds connecting the neighbouring cells is applied to represent the microstructure of cement paste, where unhydrated cement particles are placed on each site and pores of different sizes are assigned to bonds according to the measured microstructure features. The simulated microstructure of cement paste is then subjected to different loading conditions. The fracture process and damage evolution are simulated by removing failed bonds. A series of statistical analyses is performed to quantitatively investigate the effects of pore spatial distribution, porosity and pore size distribution on macroscopic mechanical properties and damage evolution. The simulation results are compared with the available experimental data.

2. 3D microstructure of cement paste

This work is focused on pure Portland cement paste without any interfacial transition zone between aggregate and matrix. The microstructure evolution of cement paste due to cement hydration was investigated by using a non-destructive technique, X-ray micro-computed tomography, which is different from other traditional experimental approaches, e.g. optical microscope and scanning electron microscope where sample preparations, such as polishing and drying, may damage the microstructure. Based on a series of image processing and analyses, pore size distribution and particle size distribution of anhydrous cement grains were measured. Details of the extraction techniques are given in the following three sub-sections.

2.1. X-ray micro-computed tomography data

The specimen used here was prepared using ASTM type I Portland cement. The w/c ratio of cement paste specimen is 0.5. After drill mixing in a plastic beaker, small parts of the paste were poured into the syringe and then injected into a micro circular plastic tube with an internal diameter of 250 μm. The micro plastic tube filled with cement paste was sealed and cured under standard conditions until testing. The specimen was scanned at curing ages of 7 and 28 days using a high resolution Xradia MicroXCT-200 CT machine at the Beckman Institute for Advanced Science and Technology at University of Illinois at Urbana-Champaign (UIUC, USA), operating at 50 keV/10 W. The X-ray shadow projections of specimen were digitized as 2000×2000 pixels with a resolution of 0.5 μm and were processed to obtain reconstructed cross-section images using the algebraic method implemented in the Xradia reconstruction software. This resulted in a 3D stack of virtual sections, each consisting of 512×512 voxels with a linear X-ray attenuation coefficient, displayed as an 8-bit image with grey scale values from 0 (black) to 255 (white).

Fig. 1 shows the micro-CT image of a cylinder region with 200 μm in diameter and 100 μm in thickness extracted from the reconstructed 3D image of the 28 days old cement paste. From Fig. 1 some characteristics of cement paste components can be seen. The darkest phases correspond to pores. The brightest phases are anhydrous cement grains. Hydration products are shown as grey.

2.2. Image segmentation

X-ray micro-CT images are composed of voxels, each of which has a unique grey scale value. Prior to morphometrical analysis of the micro-CT images, image segmentation was carried out to identify different phases in hardened cement paste, i.e. pore, hydration product and anhydrous cement grain. A large number of segmentation techniques are available in literature. The most used one is to define a global threshold value based on the grey-level histogram [7]. Voxels that have grey scale values lower or higher than the defined threshold value are considered as

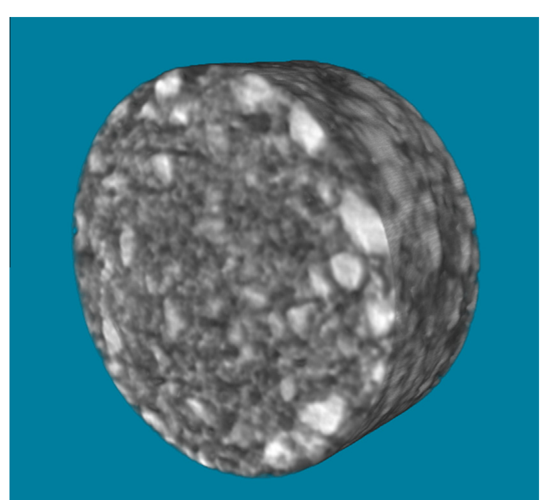

Fig. 1. Micro-CT image of the 28 days old cement paste.