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Micromechanical modelling of deformation and fracture of hydrating cement paste using X-ray computed tomography characterisation

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ABSTRACT

Cement paste is the basic but most complex component in cement composites, which are the dominant construction material in the world. Understanding and predicting elastic properties and fracture of hydrating cement paste are challenging tasks due to its complex microstructure, but important for durability assessments and life extension decisions. A recently proposed microstructure-informed site-bond model with elastic-brittle spring bundles is developed further to predict the evolution of elastic properties and fracture behaviour of cement paste. It is based on microstructural characteristics of hydrating cement paste obtained from X-ray computed microtomography (micro-CT) with a spatial resolution of 0.5 μm/voxel. Volume fraction and size distribution of anhydrous cement grains are used to determine the model length scale and pore-less elasticity. Porosity and pore size distribution are used for tuning elastic and failure properties of individual bonds. The fracture process is simulated by consecutive removal of bonds subjected to surface energy based failure criterion. The stress–strain response and elastic properties of hardened cement pastes with curing ages of 1, 7 and 28 days are obtained. The simulated Young's modulus and deformation response prior to peak stress agree very well with the experimental data. The proposed model provides an effective tool to evaluate time evolution of elastic properties and to simulate the initiation, propagation, coalescence and localisation of micro-cracks.

1. Introduction

Cement composites are the most popular and widely used construction material in the world. The understanding and prediction of elastic properties and fracture behaviour of such material are of significant technological importance and scientific interest, as they play a crucial role in the durability assessments and life extension decisions of reinforced concrete structures. The time evolution of elastic properties and fracture of such material are complicated since they strongly depend on its heterogeneous and multiphase microstructure, which generally ranges over several length scales from nanometres to metres and develops over time as a result of continued hydration of the cement [1]. At meso-scale, concrete can be considered as a three-phase composite consisting of aggregate, bulk cement matrix and interfacial transition zone (ITZ) between them. ITZ is actually a “special” cement paste with higher porosity and larger pores relative to the bulk cement matrix [1,2]. Therefore, as the most complicated and basic component in cement-based materials, the mechanical properties and fracture of cement paste accounting for microstructure should be studied in detail firstly.

Because of its significance, a lot of efforts, both experimentally and numerically, have been made to study the evolution of elastic properties and cracks of hydrating cement paste in the past decades. Among them, micromechanical modelling approaches show a great advantage because some main microstructure information can be taken into account. These approaches can be classified into three general categories: analytical models, continuum-based numerical models and discrete lattice models.

With respect to analytical models, Bernard et al. [3] proposed a multistep micromechanics homogenization approach based on effective medium approximation scheme in combination with a kinetics model of the four main hydration reactions of ordinary Portland cement to predict the time evolution of elastic properties

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of cement paste. Cement paste is regarded as a composite of calcium-silicate-hydrate (C–S–H) matrix with large calcium hydroxide (CH) crystals, cement clinker inclusions and pores, which have different mechanical properties. Based on the same procedure, Constantinides and Ulm [4] estimated the effect of two types of C–S–H, i.e., high-density C–S–H and low-density C–S–H, on the macroscopic elastic properties of hydrating cement paste with water-to-cement (w/c) ratio of 0.5 in a quantitative manner. Sanahuja et al. [5] developed a similar homogenization scheme to estimate the evolution of effective elastic moduli of hydrating cement paste that is modelled as a four-phase material made up of anhydrous cement grains, inner hydration products surrounding the anhydrous particles, outer hydration products and pores. The simulated Young's moduli of cement paste during hydration were in excellent agreement with the experimental results available in the literature. Zheng et al. [6] and Zhao and Chen [7] predicted the elastic moduli of hardened cement paste at various curing ages with various w/c ratios by using a simple three-step analytical homogenization scheme. In this scheme, hardened cement paste is modelled as n-layer composite including spherical unhydrated cement particles, C–S–H, CH and capillary pores. Pichler and Hellmich [8], and Pichler et al. [9] modelled cement paste as a two-phase composite material composed of hydrate foam and spherical cement inclusions, and used the Mori-Tanaka (M-T) [10] scheme to determine the effective elastic moduli of cement paste, which are considered as input to further investigate the mechanical properties of mortar. Although analytical models are able to provide simple expressions for estimation of elastic properties of cement paste, the proposed simplified multiphase or n-layer cement hydration models need further validation prior to applications of them.

Regarding continuum-based numerical models, finite element method (FEM) is the most widely used one. Haecker et al. [11] utilised a computer-based cement hydration model, CEMHYD3D [12], to generate the 3D digital microstructure of cement paste consisting of unhydrated cement, hydration products and pore space, and then quantitatively predicted the elastic moduli of cement paste as a function of degree of hydration by using three-dimensional (3D) FEM. The required individual phase moduli were obtained from literature. Smilauer and Bittnar [13] predicted the elastic properties of hydrating cement paste by combining the CEMHYD3D model, percolation theory and finite element analysis. The size of the representative volume element (RVE) of cement paste was found to be $50 \times 50 \times 50$ μm. Similarly, a combination of CEMHYD3D model and FEM was applied to estimate the evolution of effective elastic modulus and diffusion coefficient of cement paste with w/c ratio of 0.4 during hydration [14–16]. Hain and Wriggers [17] obtained the 3D microstructure of hardened cement paste from X-ray computed microtomography (micro-CT) with a spatial resolution of 1.0 μm/voxel and carried out microstructure-based modelling of effective elastic properties of cement paste via homogenization. A series of numerical-statistical analyses were performed to determine the RVE size for measuring elasticity of cement paste. Recently, Huang et al. [18] proposed a statistical numerical homogenization procedure through FEM to study the effective elastic properties of cement paste based on X-ray micro-CT images with a resolution of 0.95 μm/voxel. The mean values of the simulated elastic properties were in good agreement with the experimental data. Although the continuum approach is capable of predicting the mechanical properties of cement paste based on microstructure, it is inherently incapable of dealing with fracture process in cement paste, e.g., crack initiation, propagation and coalescence. In addition, the spatial resolution of X-ray CT was limited to 1.0 μm that is not high enough to obtain a realistic microstructure of cement paste. Therefore, X-ray CT with a higher resolution is required.

In regard to discrete lattice models, they offer a promising modelling strategy to investigate the mechanical properties and explain fracture processes in cement paste because of its unique feature of representing a material by a lattice system of beam or spring elements [19]. Qian et al. [20] further developed and applied the lattice beam model proposed by Schlangen and van Mier [21] based on the simplest regular lattice with cubic cells to predict the mechanical properties and fracture of hydrating cement paste. The used 3D microstructures of cement pastes at different curing ages were simulated by using a cement hydration model, HYMOSTRUC3D [22–25]. However, the simulated stress–strain response of cement paste under uniaxial tension seems too brittle and remains not realistic [26]. Additionally, this lattice model is not physically realistic in terms of shape of the represented phases in cement paste and unable to provide a linear elastic response with an appropriate elastic modulus and Poisson's ratio [27]. To overcome such limitations, Jivkov and Yates [27] proposed a novel bi-regular lattice beam model based on truncated octahedral cells, namely, site-bond model, to study the elasticity of solids and further successfully utilized to predict the mechanical behaviour, and micro-crack population and damage evolution in cement-based materials considering microstructural characteristics [19,28]. Nevertheless, this model has a shortcoming that the relationship between the global elasticity and properties of local beam elements cannot be analytically derived [29]. In order to improve this aspect, Zhang and Jivkov [29] reformulated the site-bond model by replacing beam elements with spring elements and predicted the damage evolution in hardened cement paste.

The main purpose of this work is to further develop the proposed site-bond model and apply it to simulate the elastic properties and fracture behaviour of hydrating cement paste taking into account its microstructural information. The microstructural characteristics, such as pore size distribution, porosity, and volume fraction and size distribution of anhydrous cement grains are derived from high-resolution X-ray micro-CT images along with a series of image processing and analyses. The 3D microstructure of cement paste comprised of anhydrous cement grains, hydration products and pores is represented by an assembly of truncated octahedral cells with sites at cell centres and bonds linking the neighbouring cells. The simulated site-bond assembly is then subjected to uniaxial tensile loading and stress–strain response of cement paste is obtained. The fracture process is simulated by the removal of failed bonds. The simulation results are compared with the available experimental data.

2. Microstructural characterisation of cement paste using X-ray micro-CT

2.1. X-ray micro-CT imaging

The 3D microstructure of hardened cement paste used in this work was obtained from X-ray micro-CT scans. ASTM type I Portland cement was used. The w/c ratio of the cement paste specimen was 0.5 (mass ratio). After drill mixing in a plastic beaker, small parts of the paste were poured into the syringe and then injected into a micro plastic tube with an internal diameter of 250 μm. The specimen was stored in the standard curing room with a relative humidity of 95% and temperature of 20 °C and scanned at 1, 7 and 28 days. A high resolution Xradia MicroXCT-200 CT scanner at the Beckman Institute for Advanced Science and Technology at the University of Illinois at Urbana–Champaign was used for acquiring projection images with a source power of 10 W at 50 kV. The sample was rotated on the stage from −91° to 91° at an increase of