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Random field finite element models with cohesive-frictional interactions of a hardened cement paste microstructure

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ABSTRACT

Cement paste is a disordered material whose properties and structure differ spatially and cannot be precisely predicted. We propose a new approach for developing finite element models of a hardened microstructure that accounts for the stochastic nature of cement paste. The initial model configuration is a random field that is generated according to probability density functions measured through nanoindentation experiments on samples composed of Portland cement and a volcanic ash additive. We study the influence of cohesive-frictional interactions through a Mohr-Coulomb yield criterion applied to the finite element constitutive relations. An ensemble of microstructures are simulated to assess the influence of spatial fluctuations and plasticity on the mechanical response to compressive loading. Our results indicate that the micron-scale morphology has a limited influence on the macroscopic strength behavior. These findings suggest that the shear strength scaling and dilatant behavior of cement paste originates within nanometer-scale features of the composite.

1. Introduction

Cement paste is the matrix phase in cementitious materials which include mortar and concrete. It is a heterogeneous composite that changes over time according to dynamic hydration processes that makes the precise prediction of the evolving material intractable. These complexities have limited the ability of researchers to systematically study the connection between macroscopic properties and details of the cement paste microstructure. This understanding is critical for assessing the impact of additives on engineering properties to reduce our dependence on ordinary Portland cement (OPC) mixtures and to achieve more durable and sustainable cementitious materials (Palkovic et al., 2016).

The main challenge for developing realistic cement paste models is generating the initial microstructure configuration. One approach is to simulate the hydration and growth of the microstructure according to a empirical kinetics model (Bentz, 1997; Bishnoi and Scrivener, 2009; Van Breugel, 1991). These models have been applied to predict elastic properties as a function of water-to-cement (w/c) ratio (Haecker et al., 2005) and degree of hydration (Bittnar, 2006), as well as failure behavior under tensile loading (Nguyen et al., 2012; Qian et al., 2017). Another method is to directly image the three-dimensional structure using computer-tomography (CT) scans of a hardened sample (Hain and Wriggers, 2008). This procedure provides a mapping of local densities within the material, which can be partitioned into regions of homogeneous

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properties based on assumed gray-scale thresholds (Gallucci et al., 2007). Unlike these methods which explicitly consider an initial microstructure configuration, continuum micromechanics can predict macroscopic properties according to an idealized morphology and prescribed interactions. Micromechanical models have been used to predict elastic (Bernard et al., 2003; Sanahuja et al., 2007) and compressive strength behavior (Pichler and Hellmich, 2011; Pichler et al., 2009) in agreement with experiments.

These prior studies have relied on the generation of a representative microstructure that is partitioned into a number of phases, or regions of the microstructure with homogeneous mechanical properties. The phases considered range from a detailed accounting of multiple hydrated and clinker components, to generalized domains of homogenized hydrated and anhydrous materials. The interactions within the phase are input as averaged values from published nanoindentation (Mondal et al., 2007), resonance frequency (Velez et al., 2001), or atomistic simulations (Wu et al., 2011). This traditional approach cannot account for the stochastic nature of cement paste, where microscopy (Diamond, 2004; Scrivener, 2004), chemical area mapping (Durdziński et al., 2015), and grid nanoindentation studies (Ulm et al., 2010) have shown that the microstructure exhibits significant spatial fluctuations in density and composition that can vary from a few nanometers to several millimeters. The main limitation for these methods is an inability to systematically account for variations that are fundamental to the disordered nature of the material. The question remains as to what is the influence of spatial fluctuations in microstructure morphology on the overall mechanical performance of a hardened cement paste, and how can realistic distributions describing the material heterogeneity be incorporated within model configurations?

In this work, we propose a new method for developing representative microstructures through random field finite element models. A large volume of nanoindentation experiments are performed on a hardened cement paste to measure the elastic-plastic response of approximately micron-sized regions of the microstructure. This material volume is used to define the resolution of individual elements that make up the numerical domain. The model configuration is then generated from probability density functions (PDFs) that are fit to the statistics of mechanical properties obtained from nanoindentation tests. This procedure provides a flexible approach to develop representative microstructures from a direct characterization of a hardened sample. This process also allows the size of spatial fluctuations in the microstructure to be controlled through an isotropic correlation functions used to generate the random field. To assess the influence of microstructure morphology, an ensemble of models with the same distribution of properties but varying initial configurations can be simulated with traditional finite element methods. We test our methodology by developing microstructure models of blended cement paste systems incorporating various amounts of volcanic ash (VA) as an additive in partial replacement of Portland cement.

To capture the inelastic behavior of cement paste under compression and shear loading, we use a cohesive-frictional strength envelope within our microstructure models. A cohesive-frictional material exhibits a maximum shear strength that is dependent on the magnitude of external pressure or normal-stress applied to the material (Nedderman, 2005). Compared to a purely cohesive material with the same strength under pure shear loading, a cohesive-frictional material will exhibit an increased strength and resistance to plastic deformation when external confinement is applied. Macroscale triaxial loading experiments on cm-sized cement paste samples (Heukamp et al., 2001), nm-scale modeling of calcium-silicate-hydrate (C-S-H) colloidal assemblies (Palkovic et al., 2017a) and atomistic modeling of molecular C-S-H interfaces (Palkovic et al., 2017b) have indicated that cement paste exhibits cohesive-frictional behavior at multiple length scales. However, to the authors' knowledge, no existing study of cement paste at the microstructural scale has considered a cohesive-frictional plasticity model to describe the large deformation response.

This paper is organized as follows. In Section 2 we provide an overview of nanoindentation experiments that are used to assess elastic-plastic properties of homogeneous microstructural regions within a hardened cement paste. We also propose a method of analyzing nanoindentation results to obtain PDFs of mechanical properties that can be input within existing random field modeling techniques. Section 3 describes our methodology for generating random field realizations using the measured mechanical property PDFs, and how appropriate constitutive relations are applied for implementation within a finite element model. In Section 4, our microstructure models are subjected to uniaxial compression with varying magnitudes of lateral confinement to study the material response under multiaxial stress. Finally, in Section 5, we compare our numerical results with larger-scale microindentation and cm-scale uniaxial compression experiments.

2. Measuring statistical distributions of mechanical properties

This section describes the application of nanoindentation experiments to measure the statistical distribution of mechanical properties within a cement paste microstructure. This data is analyzed to determine representative PDFs that can be incorporated within random field models.

2.1. Materials

We investigate cement paste mixtures incorporating Portland cement and volcanic ash (VA). Our mixes have a water to cement (w/c) ratio of 0.35 and consist of 0%, 10%, and 30% of VA substitution for Portland cement that we designate OPC, VA10, and VA30, respectively. A detailed characterization of the raw Portland cement and VA materials is published elsewhere (Kupwade-Patil et al., 2016). All samples were prepared according to ASTM C 305 (2014), cured for 28 days, and then inserted into acetone to retard hydration. Three samples of each mix combination were cured in 5 cm cubic molds for