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Combined meso-scale modeling and experimental investigation of the effect of mechanical damage on the transport properties of cementitious composites

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ABSTRACT

The transport properties of cementitious composites such as concrete are important indicators of their durability, and are known to be heavily influenced by mechanical loading. In the current work, we use meso-scale hygro-mechanical modeling with a morphological 3D two phase mortar-aggregate model, in conjunction with experimentally obtained properties, to investigate the coupling between mechanical loading and damage and the permeability of the composite. The increase in permeability of a cylindrical test specimen at 28% aggregate fraction during a uniaxial displacement-controlled compression test at 85% of the peak load was measured using a gas permeameter. The mortar's mechanical behavior is assumed to follow the well-known compression damaged plasticity (CDP) model with isotropic damage, at varying thresholds, and obtained from different envelope curves. The damaged intrinsic permeability of the mortar evolves according to a logarithmic matching law with progressive loading. We fit the matching law parameters to the experimental result for the test specimen by inverse identification using our meso-scale model. We then subject a series of virtual composite specimens to quasi-static uniaxial compressive loading with varying boundary conditions to obtain the simulated damage and strain evolutions, and use the damage data and the previously identified parameters to determine the evolution of the macroscopic permeability tensor for the specimens, using a network model. We conduct a full parameter study by varying aggregate volume fraction, granulometric distribution, loading/boundary conditions and "matching law" parameters, as well as for different strain–damage thresholds and uniaxial loading envelope curves. Based on this study, we propose Avrami equation-based upper and lower bounds for the evolution of the damaged permeability of the composite.

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1. Introduction

It is now common knowledge that the transport properties of a cementitious composite, i.e.; permeability and chloride diffusion coefficient, are important indicators of its durability. These composites are porous and basic, and the characteristics of its pore network, dimensions and interconnectivity of the capillarity porosity determine the transfer of aggressive species inside the matrix [1,2]. A perusal of the available literature on the subject reveals myriad studies, mostly experimental, on the different factors influencing the permeability and diffusivity of the *undamaged* composite, for example, mix parameters, moisture content and environmental conditions such as sulphate attack [3]. As a general rule of thumb, a reduction in volume, size, and inter-connection of pores will reduce the permeability and diffusivity. A reduction in pore characteristics can be achieved by selecting appropriate aggregates or cement paste properties. Reducing the amount of water relative to the cementitious material used can lead to improved pore formation. However, while the transport properties of the undamaged composite are associated with the overall porosity and the size/stability of the voids in it, the transport properties of the same composite material under load, i.e. *damaged concrete*, depend heavily on the cracks present. The formation and propagation of cracks in such composite structures is one of the major factors influencing the transport properties and thus their durability. Cracks accelerate the penetration of water and the diffusion of harmful ions, such as chloride, leading to damage and durability problems [10]. Therefore, predicting the behavior of the damaged composite using only the data for the undamaged material is pointless and there is a clear need to study the evolution of transport properties in cementitious composites with stress-induced damage.

The relationship between the mechanical properties and the permeability of cementitious composites has been under investigation

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over the last few decades. Choinska et al. [4] investigated the coupled problem of mechanical damage in concrete and its permeability and concluded that for low to intermediate levels of stress, the permeability appears to increase drastically as the load approaches the ultimate compressive strength (UCS) of the material. Samaha et al. [5] confirmed the presence of micro-cracks during uniaxial compression loading up to about 70% of the UCS, but found that the transport properties were largely unaffected. In this phase, the composite showed 15–20% less resistance to fluid and ion movement. Picandet et al. [6] found that a load of 90% of the UCS created an inter-connected network of micro-cracks which increased the gas permeability of concrete even after complete unloading. The permeability measured to chlorides follows the same behavior for the loads over than of 80% [7] or 90% of the peak [8]. The repeat of a compression load between 60 and 80% leads to an increase in the permeability as well by extension of micro-cracking. One may conclude that the interconnection of the generated micro-cracks during mechanical loading appears to be the driving factor for changes in the transport properties of a cementitious composite. Picandet et al. [9] experimentally studied the effect of a crack on the gas and water permeability of cementitious composites and found that both gas and water permeability increased proportionally to the *cube* of the crack opening displacement. Djerbi Tegguer et al. [10] performed a single cycle of compressive loading for *various loads* between 60% and 90% of the UCS. They reported that the damaged permeability increased by a factor of 10 for an increase in damage by a factor of 2.5. They also noted that gas permeability was more sensitive to damage levels than the chloride diffusivity, a result that can be confirmed by [1].

The literature clearly corroborates the experimental observation that damage, in other words, the creation and propagation of micro- or macro-cracks, leads to an increase in the value of the transport properties of a cementitious material. However, studying the effect of progressive damage on the permeability *during* continuous loading of a composite specimen experimentally, in the same manner as [10], is no easy task, requiring a great amount of time and incurring significant cost. This is where simulation-based investigation could potentially make a difference, as once sufficiently accurate material models have been established for the phenomena under consideration, and using the greatly advanced numerical tools available today, one would greatly limit the time, effort and money involved in a full-bore experimental investigation.

In addition to the above experimental studies, there have been simulation-based studies on the damage-permeability coupling in cement-based materials [11]. Chatzigeorgiou et al. [12] used a discrete lattice model to obtain this coupling. However, most of the modeling investigations typically relate the intrinsic damaged permeability with strain and isotropic damage for a homogeneous material and do not take the heterogeneity of the composite into account, with the exception of the meso–macro multi-scale approach used by Jourdain et al. [13] who considered a single crack in a homogenized domain, by solving the macroscopic moisture transport equation. There is, in our opinion, a dearth of literature on modeling-based investigation that couples local damage (distributed throughout the domain) and strain data with permeability for a cementitious i.e. heterogeneous composite with multiple phases, under *progressive* load.

Cementitious composites are typically heterogeneous brittle materials that are known to fracture through the formation, growth and coalescence of micro-cracks [14]. Failure processes in concrete depend on the loading rate and are significantly influenced by micro-inertia of the material adjacent to a propagating micro-crack and moisture in the capillary pores.

These phenomena demonstrate the involvement of multiple length scales at different levels in the mechanical response [15] as well as transport behavior of the composite. The smallest length scale is associated with the microstructure (cement paste) composed of water, hydrates (mainly C–S–H, Portlandite CH or Ettringite [16]) and anhydrous cement grains. The meso-scale is divided into a sub-meso-scale where the mortar is considered to be constituted by sand particles embedded in a homogeneous cement paste, and a meso-scale itself representing concrete as a two or three phase composite material (mortar matrix and aggregates with or without an Interfacial Transition Zone or ITZ [17]).

A realistic numerical simulation of material behavior must adequately represent the influence of as many of these length scales as possible on the mechanical and hygral response. Purely macroscopic models that do not consider the mesoscale or microstructural interactions miss out on critical information on local variables (like damage and strain) that renders them nearly useless in problems related to durability. Lattice models have been successfully used [18,19] but the results obtained appear to be lattice geometry-dependent. On the other hand, *mesoscopic modeling* with a regularized continuum description using a multiphase composite model along with matrix–inclusions interaction, in conjunction with a regularized model for the bulk material, is a safe and effective approach for characterizing the effects of the different length scales on the composite's mechanical and transport behaviors. These models provide a good balance of low computational effort and sufficient reliability. The recently contributed exact solutions in [20,21] for general heterogeneous materials and by Barretta et al. [22,23] for Functionally Graded Materials (FGMs) could be useful for comparison with FE computations on the type of composites considered here.

Since mesoscopic modeling of the composite is ostensibly the way to go, a sufficiently detailed morphological model for the mortar-aggregate composite is the next step. The mortar phase may be described as a partially saturated open porous medium with an isotropic permeability tensor under zero load. This tensor can dramatically change when load is applied due to the strain/damage dependence of the intrinsic permeability (as has been discussed in the earlier paragraphs of this section). As far as the aggregate phase is concerned, one needs to take into account their mineralogical nature, morphology, granulometric distribution and volume fraction. Depending on the type of aggregate (siliceous, plastic, calcareous) *ergo* texture (rough/smooth) [24] one can expect varying levels of bonding to the mortar phase [25], and have angular or rounded shapes [26], and of course volume fraction and gradation [27–29] all of which can significantly modify the stress distribution and thus the damage distribution within the mortar phase [30] and thus contribute to wildly varying transport parameters (e.g. permeability) of the whole composite.

The next aspect of the generation of meso-structures with random morphologies involves varying the shape, size distribution and volume fraction of the chosen aggregate particles. The literature shows 2D representations with circles/polygons [31,15,32], 3D analyses with spherical representations [25,33,30,34,26], realistic particles [35,26,36] and even considered the phenomenon of aggregate segregation due to elevated fluidity [26]. Finite Element mechanical analysis of the created mesostructures could use conforming/non-conforming meshes with tetrahedral [26] or cubic elements [37].

The mechanical constitutive behavior of the cement mortar (strain softening) for the selected shape, size and fraction of the aggregate particles with type-dependent interaction between the phases is the next important aspect since this alone can cause significant variation in the results obtained. Depending on the type of loading, either brittle failure or viscoelastic rate-dependent models are typically used, with a few implementations focusing on quasi-static displacement controlled loadings where plastic behavior may be observed. An additional step involves selection of an appropriate strain–damage evolution curve. The purpose of this

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