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Towards a realistic morphological model for the meso-scale mechanical and transport behavior of cementitious composites

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ABSTRACT

In this work, we investigate the mechanical and transport properties of cementitious composites using a realistic morphological 3D matrix-inclusion-ITZ model for the mesoscale behavior. Assuming a compression damaged plasticity-based behavior for the matrix phase under quasi-static loading, the model is used to determine the effect of inclusion (aggregate) shape, volume fraction and segregation on the mechanical response of the composite specimen under uniaxial loading. We then use the model to evaluate the effect of the previously mentioned variables as well as aggregate intrinsic permeability on the macroscopic permeability of the same composite specimen using a series of non-conforming FE meshes and level set functions to monitor the heterogenities. The model is then applied to a self-compacting concrete (SCC) with a higher volume of cement paste in order to flow more freely and be formed into complex shapes without shaking. However, this elevated fluidity predisposes SCCs to a higher risk of segregation, i.e. separation between the suspending phase and coarse aggregates, which can affect the mechanical behavior of the composite.

1. Introduction

A cementitious composite is essentially a heterogeneous brittle material that fractures through the formation, growth and coalescence of microcracks [1]. Failure processes in these composites depend on the loading rate and are significantly influenced by micro-inertia of the material adjacent to a propagating microcrack and moisture in the capillary pores. Modeling of failure and fracture in cement-based composite materials is one of the fundamental issues in structural mechanics [2].

These phenomena show that the mechanical response of such a composite involves multiple length scales defined at various levels [3]. The smallest length scale may be associated with the microstructure (cement paste) composed of water, hydrates (mainly C—S—H, Portlandite CH and hydrated sulfoaluminates) and anhydrous cement grains. The meso-scale is divided into a sub-mesoscale where the mortar is considered to be constituted by sand particles embedded in a homogenous cement paste, and a mesoscale itself representing the material as a two or three phase composite: mortar (matrix) and coarse aggregate (inclusions) with or without an Interfacial Transition Zone or ITZ).

A realistic numerical simulation of material behavior must adequately represent the influence of as many of these length scales as possible on the mechanical response. Purely macroscopic models that do not consider the mesoscale or microstructural interactions usually lose vital information [4,5], for example, in problems related to durability. Lattice models have been used with some success [6,7] but they appear to have a major drawback in that the results obtained show a strong dependence on the lattice geometry considered. On the other hand, a mesoscopic model based on a regularized continuum description using a two or three-phase composite model taking matrix-inclusion interaction into account, coupled with a regularized model for the bulk material, is an effective approach for the characterization of the effects of the different length scales on the mechanical behavior. These models also present an excellent compromise between the computational effort involved and reliability of the result obtained.

Mesoscopic modeling of these materials needs a sufficiently accurate morphological model for the mortar-aggregate composite. The mortar phase may be described as a partially saturated porous medium. Aggregates are characterized by their mineralogical nature together with their morphology (shape) and granulometry (size distribution). These aggregates may be of different types

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(siliceous, plastic, calcareous and even ceramic [8]) and having different textures (rough or smooth) [9] as a result having different levels of bonding to the mortar [10], and have an angular and elongated or rounded and compact shape, all of which can have a significant influence on the stress distribution within the concrete material [8,11] and thus contribute to differences in mechanical and transport behavior of the final formed composite. In addition, the aggregate volume fraction and gradation have an effect on the mechanical performance [12,13].

This means that in the generation of random composite mesostructures the shape of the inclusions, i.e. aggregate particles has to be taken into account in order to study the effect of aggregate shapes upon the mechanical behaviour of the final material. A survey of the existing literature shows numerous implementations of mesoscopic modeling of cementitious composites, and these generally focused on two main issues: the first being the morphological representation of the composite at the mesoscale, and the second related to the strain softening behavior of the cement mortar. Most have focused on either 2D representations using either circles or polygons [14,3], and the papers involving a full bore 3D analysis have been limited mostly to spherical representations, arranged in a regular [10] or random fashion [15,11,16]. One of the most recent contributions involved using realistic particles instead of the traditional spherical shapes in a mortar-aggregate model by Refs. [17], who used a spherical harmonic expansion to represent irregular shapes, followed by a take-and-place parking method to place these particles in the matrix. [18] used a 2D Voronoi algorithm to represent a general heterogenous material for dynamic brittle crack propagation simulation.

Numerical analysis of the thus-created heterogeneous materials using the FEM requires the discretisation of the created mesoscopic models. Different meshing techniques have been applied for the discretisation of complex microstructures including conforming and non-conforming meshes by using a projection of a uniform mesh into the heterogenous material, as well as cubic meshes with an increased number of integration points [19].

[20–23] recently contributed exact solutions for Functionally Graded Materials (FGMs) (that bear a resemblance to the type of composites studied in this work, especially with aggregate segregation) that provide useful benchmarks for numerical computations on heterogenous materials.

The mechanical constitutive behavior of the cement mortar (strain softening) and the nature of interaction between the phases is another important element that 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.

In the particular case of an SCC, which is the material used in this work, the heightened fluidity of the mortar (on account of a higher than usual volume of cement paste) predisposes them to a higher risk of segregation compared to if they were vibrated, i.e. separation between the suspending phase and coarse aggregates, which can affect the mechanical and transport behavior of the prepared composite [24–26]. To the author's knowledge, there is very little existing quantitative research on the effect of aggregate segregation on the mesoscopic behavior of the composite material.

In this contribution we will perform three-dimensional analyses of quasi-static compression and tension tests of a composite specimen at the mesoscale level. We use a rate-independent isotropic inviscid plastic damage (CDP) continuum model to model the mechanical behavior of the matrix (mortar) under quasi-static loading in conjuction with an explicit morphological model for the mesostructure including aggregate grains (inclusions) embedded in a mortar (matrix) with a possible consideration of an ITZ between the two phases.

The effect of different aggregate shapes has been modeled using a random spherical representation as well as a series of non-intersecting randomly sized and oriented polytopes generated using an “exploded” Voronoi tesselation in 3D. In addition, the effect of aggregate segregation, a side-effect of the particular mortar used in this research (SCCs) has been taken into account in this mesoscale model.

The remainder of the paper is organized in the following manner: Section 2 describes the experimental setup used to determine the mechanical constitutive parameters of the cement mortar used in the study. Section 3 explains the morphological three-phase composite model used for the mesoscale description. Section 4 explains the mechanical constitutive model used for the individual phases, and Section 5 provides the results obtained after simulation with a discussion. The paper ends with concluding remarks and suggestions for future work.

2. Materials and experimental techniques

The cement mortar modeled in this paper has the composition given in Table 1. It contains sand S and has a water to binder ratio w/c equal to 0.37. A slag cement, CEM III/A 52.5L type, is used and its physical composition is given in Table 2.

A standard displacement-controlled uniaxial compression test was performed on a specimen of mortar (Fig. 1 (a)) with dimensions $40 \times 40 \times 40$ mm to obtain the Ultimate Compressive Strength (UCS), and this was then used in conjunction with the CEB-FIP Model Code 2010 to estimate the uniaxial compression test curve and thus the elastic constitutive and damage parameters for the mortar. This prevents the usual problems associated with using the experimental compression test for the complete stress–strain curve.

Aggregates are calcareous with elastic brittle behavior [9]. The mechanical properties for the two are shown in Table 3, (ρ = density, Y = Young's modulus, UCS = Ultimate Compressive Strength, and ν = Poisson's ratio).

Two SCC specimens of size $70 \times 70 \times 280$ mm were prepared – the second one with a moderate segregation of aggregates along 70% of the specimen's height for the same aggregate volume fraction – in order to demonstrate the segregation phenomenon, as shown in Fig. 2.

Finally, the permeability was measured for the mortar using the traditional gas permeability measurement (Table 3) using the set up shown in Fig. 1(b).

Table 1
Composition of the mortar used in this work.

Constituent	Composition (kg/m^3)
Cement CEM III/A 52.5L	330
Limestone filler	240
Sand S(0–0.4 mm)	780
Water	210
Superplasticizer	1.8

Table 2
Composition and physical properties of the slag cement used in this work.

Clinker	Slag	Blaine specific surface area	Specific gravity
%	%	cm^2/g	g/cm^3
36	62	4263	2.98