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A mesoscale approach for modeling capillary water absorption and transport phenomena in cementitious materials

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ABSTRACT

This paper proposes a mesoscale approach for simulating moisture transport by capillary action in partly-saturated porous cementitious composites. The modeling approach explicitly accounts for moisture transport through a mesostructure composed of coarse aggregates, surrounding cementitious mortar and interfaces. These latter, namely interface transition zones (ITZs), allow to describe the interaction between aggregates and mortar, and may cause an alternative path for the internal moisture movements. Basic morphology effects of the ITZs are simulated using a ribbon approach. Random spatial distribution of cement particles are stacked in the meso-geometry. Aggregate particles are introduced as randomly perturbed polygons and the moisture transport is modeled as a diffusion problem and solved by means of the finite element method. The proposed constitutive models are based on a proper description of the permeability and pore size distribution which strongly affect the local moisture content. Numerical results at both macro- and mesoscale levels demonstrate the soundness and capability of the proposed approach. The integrated modeling results actually demonstrate the potential of the mesoscale approach and shows the role of the ITZs as an internal interconnected network.

1. Introduction

Concrete is one of the most employed construction materials in the world, mainly due to its relative low cost and high performance. Many structures made of cementitious materials suffer during their lifetime a wide spectrum of mechanical loads and environmental conditions. In this context, concrete durability results of crucial importance and, moreover, transport processes in cementitious materials play a key role in related durability issues [1,2].

In this regard, moisture transport has a direct consequence on affecting phenomena such as chloride penetration [3,4], alkali-silica reaction (ASR) [5,6] and carbonation [7]. Furthermore, the study of moisture transport results of big importance in solidification/stabilization processes employed to contain hazardous wastes or treat contaminated areas [8]. Diffusion transport models could be actually employed for investigating the effect of different waste stream (heavy metals bearing sludge, filter cake, fly ash and slag) which alter the hydration properties of cement and/or other binders [9].

Plenty of experimental studies addressed the issue of transport phenomena and capillary diffusion in concrete materials. They emphasize the key importance of understanding the moisture transport in concrete and mortar to estimate their service life and durability. In this sense, outstanding tests of capillary water transport in concretes with different water/cement ratio, sand size distribution and curing were proposed by Martys and Ferraris [10]. Moreover, an experimental technique, based on gravimetric measurements of capillary water absorption, was proposed by Goual et al. [11] for investigating the water content profiles and the isothermal capillary transport coefficient in a series of specimens.

Several theoretical models are available in the scientific literature for simulating moisture transport and diffusion processes in concrete materials [12–14]. Nonetheless, most of them deal with a macroscopic description of the medium [15,16]. Only few

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Nomenclature

B	Raleigh-Ritz pore size distribution constant [m^{-1}]	u^{+}	uplift displacement (interface) [m]
C	empirical constant for capillary pressure [–]	Δ_{θ}	difference of the hydraulic heads (interface) [m^3/m^3]
d_n	unit normal diffusivity (interface) [$m\ s^{-1}$]	ϕ	concrete open porosity [m^3/m^3]
D_t	transversal diffusivity (interface) [$m^2\ s^{-1}$]	γ_{lv}	liquid-vapor interfacial energy [$N\ m^{-1}$]
D_{θ}	capillary diffusivity (continuous) [$m^2\ s^{-1}$]	μ	water dynamic viscosity [$N\ s\ m^{-2}$]
K_{θ}	unsaturated water permeability [$m^4\ N^{-1}\ s^{-1}$]	$\nabla\cdot$	divergence tensor operator [–]
p	pore pressure [$N\ m^{-2}$]	∇	gradient tensor operator [–]
q_n	normal fluid flow (interface) [$m\ s^{-1}$]	θ	water content [m^3/m^3]
q_t	transversal fluid flow (interface) [$m\ s^{-1}$]	θ^{+}	water content at the master side of the discontinuity (interface) [m^3/m^3]
q^{in}	positive leak-off rate in the transverse flow (interface) [s^{-1}]	θ^{-}	water content at the slave side of the discontinuity (interface) [m^3/m^3]
q^{out}	negative leak-off rate in the transverse flow (interface) [s^{-1}]	θ_c	liquid-solid equilibrium contact angle [°]
t	time [s]		

proposals account for lower scales of observation and description of the problem. As references, it can be first cited the work by Segura and Carol [17] who proposed a formulation for diffusion problems through discontinuities. They superimposed line elements onto the standard continuum discretization by means of single, double or triple node interface elements suitable for the micro- and mesoscopic longitudinal and transversal fluid flow. Huang et al. [18] presented a model which captures the moisture transport in concrete based on pore size distribution, represented by means of a multi-Rayleigh-Ritz model which includes microcracks, gel pores, small and large capillaries. An interesting formulation, to solve the coupled hydro-mechanical behavior by means of zero-thickness interface elements, was also proposed by Segura and Carol [19]. Furthermore, Schlangen et al. [20] investigated, at mesoscale level, the influence of the water content on the effect of drying shrinkage, cracking response, tensile strength and ductility issues.

It is worth noting that only very few papers were found in the scientific literature modeling water diffusion phenomena in partially saturated concrete media at the mesoscale level. In this matter, the work by Wang and Ueda [21] should be mentioned, who proposed a 2D lattice-based model for analyzing the water penetration into unsaturated concretes at the mesoscale level. A further extension of this approach to a 3D analysis was proposed by Abyaneh et al. [22]. In both cases the hydraulic diffusivity was simply schematized through an empirical exponential negative law rule based on the degree of saturation.

In the current study, the concrete mesostructure, i.e. matrix and ITZ between matrix-aggregate, is explicitly modeled. With this, the outcome of simulations was employed to evaluate the predominance of possible moisture movements through either the matrix (diffusion) or ITZ (capillary action). The proposed model uses the extended Darcy's law to simulate moisture transport, where the capillary (pore) pressure is explicitly considered and affects both the matrix diffusivity as well as the ITZs. Aggregate particles are explicitly modeled in the mesoscale approach by means of classical iso-parametric finite elements. From there, particle-matrix interfaces (ITZs) are schematized by combining zero-thickness interface and pipe elements. Originally, these elements allow both normal and transversal diffusivity among the joints in a mesoscopic analysis. Main objective of this proposal is, therefore, to develop a novel mesoscale approach for modeling the capillary water absorption and internal transport phenomena in cementitious media, while taking into account the diffusivity and capillary action in the ITZs as the main drivers. The key results of this study deal with examining and numerically quantifying the effect of the ITZs on the water absorption and internal moisture transport of cementitous materials, like concrete or mortars. An original mesoscale approach, having relatively low computational costs, easy to be implemented in classical FE environments and based on Voronoi-Delaunay tessellation arrangements of aggregates, is proposed.

After this general introduction about the State-of-the-Art and main motivations of this research, the paper is organized as follows. Section 2 reports the general formulation and assumptions of the mesoscale model formulation. Diffusivity rules and constitutive models, to analyze moisture diffusion and capillary water absorption phenomena in both mortar and concrete substrates, are outlined in Section 3 (continuous description) and Section 4 (discontinuous or ITZ description). Then, Section 5 proposes the model validation, reporting some comparisons of a series of experimental results available in the scientific literature and assumed as benchmark, against the corresponding numerical simulations. Finally, some concluding remarks and future research lines will be described in Section 6.

2. Mesoscale modeling

The mesoscale moisture diffusion analysis is presented in this section. The 2D geometry generation procedure of concrete mesostructure is next highlighted.

A convex polygonal geometrical technique is adopted for representing coarse, medium and small aggregates, which are then immersed into the surrounding mortar matrix. Particularly, the polygonal geometry is numerically generated through standard Voronoi/Delaunay tessellation [23,24] starting from a regular array of points (Fig. 1a) which are slightly perturbed as shown in Fig. 1b. Then, the generated Voronoi convex polygons (1c) are percentually resized and randomly rotated as shown in Fig. 1d. The detailed description of these operations are out of the scope of this work, but further details can be found in [25].

In order to generate the geometric model for analysis, the polygonal particles and the space between them (i.e., surrounding matrix) are meshed with isoparametric continuum Finite Elements (FEs). Then, zero-thickness interface elements and pipe elements are inserted throughout the adjacent edges of the coarse and surrounding mortar elements. Nonlinear moisture diffusion rules are introduced in those interface elements according to the formulation outlined in the following Sections 3 and 4. The moisture movement, for mortar and aggregates, which are discretized by means of isoparametric FEs, follows a nonlinear diffusion-type equation for unsaturated media which is presented in Section 3. Then, fluid flow through ITZs between cementitious mortar and aggregates is proposed through the formulation of normal and longitudinal (or