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Computational homogenization of cement paste: influence of microstructure model parameters on mechanical properties

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Abstract

Cement paste serves as a binder for cementitious materials and plays a crucial role in the production of construction materials. The microstructure of cement paste, developed during the hydration process, generally consists of a mixture of different hydration products, unreacted clinker particles, and pores. The microstructure-informed micromechanical modeling of cement paste is becoming increasingly popular since it links microstructural features and effective behavior at the macroscale and potentially enhances the understanding of cement paste's behavior [1]. Although experimental and numerical techniques have been proposed in the literature to generate models of the microstructure of cement paste, microstructure-informed modelling remains challenging due to the complex, multicomponent nature of this microstructure. One approach to generating a model of the cement paste microstructure involves employing computational methods to simulate the hydration process, enabling the prediction of phase volume fractions and their spatial distributions. In this study, the Virtual Cement and Concrete Testing Laboratory (VCCTL) software has been utilized. Fig. 1 shows the model of the Portland cement paste microstructure after 28 days of curing, considering the water-to-cement ratio of 0.35; each color represents a different phase, including various hydration products (e.g., calcium silicate hydrate (C-S-H), portlandite, ettringite, etc.), clinker phases (alite, belite, tricalcium aluminate, etc.), and pores. The presented model represents a 300×300×300μm volume, where each voxel measures 1×1×1μm. The numerical homogenization based on the fast Fourier transform-based (FFT) approach determines effective elastic properties. This work aims to establish a relationship between the size of the microstructure model (starting from 300×300×300μm and successively reducing its dimensions) and the effective elastic constants. Moreover, the obtained results are compared with those provided by the model generated based on the microtomographic results reported in the literature [2]. The comparison aims to verify if the hydration simulation-based microstructure models yield comparable results to experimentally obtained models.

The investigation results, which will be presented during the conference, are expected to facilitate the preparation of virtual cement paste microstructure models, allowing for achieving a balance between model simplicity and accuracy of homogenization. Subsequently, they can be employed in multiscale simulations to capture interactions across different scales. The potential application of such models within a multiscale framework has been discussed in recent work [3].

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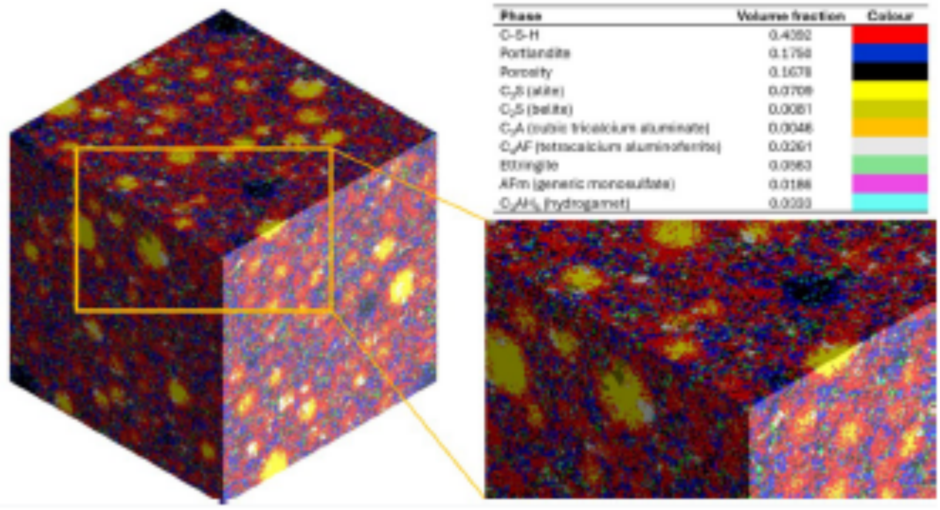

Phase	Volume fraction	Colour
C-S-H	0.4352	
Portlandite	0.1758	
Porosity	0.1678	
C_3S (alite)	0.0709	
C_2S (belite)	0.0081	
C_3A (cubic tricalcium aluminate)	0.0046	
C_4AF (tetracalcium aluminoferrite)	0.0261	
Ettringite	0.0563	
AFm (generic monosulfate)	0.0188	
C_3AH_6 (hydrogarnet)	0.0333	

Figure 1. Model of the microstructure of Portland cement paste generated based on simulation of hydration process in VCCTL software, 28 days of hydration, 300x300x300 µm

Scientific field: computational mechanics

Keywords: numerical homogenization, representative volume element, cement paste

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