26th INTERNATIONAL CONFERENCE ON COMPUTER METHODS IN MECHANICS

CMM 2025

Short Papers

Editors

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Łódź University of Technology
Faculty of Civil Engineering, Architecture and Environmental Engineering
8th - 11th July 2025, Łódź, Poland

Editors:
Marcin Kamiński, Paulina Świątkiewicz

Linguistic editing: Joanna Pawliczak
Technical editing and typesetting: Agata Niewiadomska
Cover design: Agata Niewiadomska

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ISBN: 978-83-67934-60-2

DOI: 10.34658/9788367934602

This book is published due to financial support of National Science Center in the framework of the research grant OPUS No. 2021/41/B/ST8/02432, "Probabilistic Entropy in Engineering Computations", sponsored by the National Science Center in Cracow, Poland, in the period of 2022–2025.

Lodz University of Technology Press
93-005 Lodz, 223 Wólczańska St.
Phone: 42-631-20-87, 42-631-29-52
E-mail: zamowienia@info.p.lodz.pl
www.wydawnictwo.p.lodz.pl

Lodz University of Technology Conference Proceedings, No 2586

Circulation 300 copies
Printing and bookbinding: Quick-Druk
90-562 Lodz, 11 Łąkowa St

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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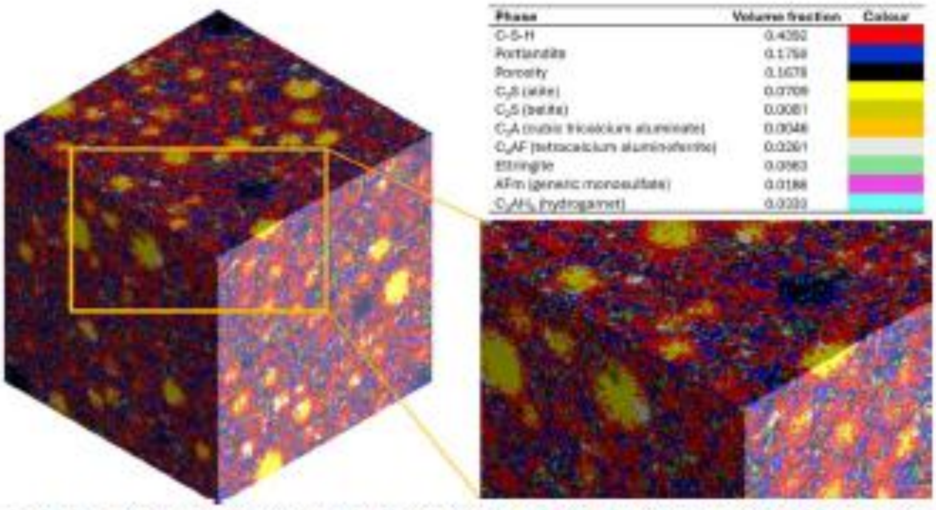

Figure 1. Model of the microstructure of Portland cement paste generated based on simulation of hydration process in VCCTL software, 28 days of hydration, 300x300x300 μm

Scientific field: computational mechanics

Keywords: numerical homogenization, representative volume element, cement paste

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