# Prediction of elastic properties of cement paste using computational homogenization: a comparison of different microstructural models

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The microstructure of cement paste, formed during hydration, is typically composed of hydration products, unreacted clinker particles, and pores. Microstructure-informed micromechanical models establish a link between the microstructure and the effective mechanical properties [1]. This study addresses the computational homogenization of cement paste, accounting for different types and sizes of representative volume elements (RVEs). Two microstructure models are considered: one based on simulations of the hydration process, and the other derived from experimental microtomographic data [2]. The hydration process is simulated using the Virtual Cement and Concrete Testing Laboratory (VCCTL) software [3]. To enable a direct comparison between the considered microstructure models, a simplified three-phase virtual microstructure is also developed [4]. A multilevel Mori–Tanaka analytical scheme is employed to perform preliminary homogenization of anhydrous cement grains and hydration products. Subsequently, the homogenization is carried out using a Fast Fourier Transform (FFT)-based method. In addition, local stress distributions at the microstructural level are analyzed for both microstructure models. For sufficiently large RVEs, good agreement is observed between the simulation-based and experimentally based microstructure models. During the conference, the influence of RVE size on effective properties, along with the differences between model outcomes, will be discussed.

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