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Uncertainty analysis in multiscale modeling of concrete based on continuum micromechanics

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ABSTRACT

Reliable models for structural materials are a vital issue. Hierarchical multiscale models for concrete, incorporating microstructural properties of the material, have been developed to predict the mechanical behavior. The present paper aims to study the major sources of uncertainty in the framework of multiscale modeling based on continuum micromechanics. The effect of uncertainy in input parameters on the Young's modulus of cement-based materials is studied systematically by means of a probabilistic multiscale modeling approach covering three length scales. Sensitivity and uncertainty analyses are adapted to assess the stochastic predictions of the multiscale model. The total order sensitivity indices are computed using the variance-based sensitivity analysis. The total uncertainty according to the adjustment factor approach, comprising the parameter uncertainty and the model uncertainty, is quantified, aiming at the comparison of two commonly utilized hydration models. Application of the probabilistic methodology reveals that the uncertainties of the model responses increase significantly during the upscaling process. Hence, considering the stochastic variability of the predicted mechanical properties is of utmost importance for the assessment and evaluation of the model responses.

1. Introduction

Multiscale models are useful for the estimation of material properties. During the last few decades, multiscale models based on continuum micromechanics have been developed and applied to cement-based materials successfully. This established the model-based prediction of their mechanical and physical properties, e.g. (Bernard et al., 2003; Constantinides and Ulm, 2004; Pichler and Hellmich, 2011; Sanahuja et al., 2007). The implementation of the continuum micromechanics based multiscale models is performed in a two-stage process: First, the evolving volume fractions of the material phases are determined using hydration models, followed by an upscaling procedure. In comparison to empirical phenomenological models that are mostly defined at the macroscale of materials, multiscale models consider the microstructure explicitly, i.e. the intrinsic elastic properties of the constituents and their volume fractions. Therefore, a large number of input parameters is required. Commonly, multiscale analyses are performed deterministically using established values for the input parameters. Nonetheless, the input parameters include inherent uncertainties which influence the predicted model responses. Calculations comprising the stochastic input parameters result in probabilistic multiscale analyses where the model responses represent stochastic variables as functions of the parameter variation. In doing so, the question of uncertainty quantification across scales during the multiscale modeling process is brought into focus.

Uncertainty quantification in mechanical models has been a matter of research for the last few years (Sudret, 2015). Uncertainty and sensitivity analyses have been already employed to quantify the stochastic variation of phenomenological models that have been developed and applied at the macroscale of cement-based materials (Madsen and Bažant, 1983; Howells et al., 2005; Yang, 2007; Keitel and Dimmig-Osburg, 2010). Particularly, creep models have been investigated intensively, e.g. sources of uncertainties in creep models have been determined (Keitel, 2013), and main influencing parameters on the model responses have been identified (Howells et al., 2005; Yang, 2007; Teplý et al., 1996). The role of uncertain input parameters has also gained much attention in the field of multiscale modeling. Clément et al

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(Clement et al., 2013). have investigated the uncertain nature of hyperelastic heterogeneous materials at the microscopic scale and have proposed a methodology for the uncertainty quantification based on polynomial chaos representation. A stochastic multiscale approach has been also used to characterize the uncertainty propagation across the length scales of polycrystalline alloys (Kouchmeshky and Zabaras, 2010) and of nanocrystalline membranes in metals (Koslowski and Strachan, 2011). Vu-Bac et al. have proposed stochastic multiscale methods for amorphous polyethylene (Vu-Bac et al., 2014) as well as for polymer nanocomposites (Vu-Bac et al., 2015), aiming at the identification of influencing key parameters on the Young's modulus. The uncertainty propagation across four length scales under consideration of correlated input parameters has been studied (Vu-Bac et al., 2015). Uncertainties in the multiscale modeling of concrete have been rarely investigated so far. Venkovic et al. have computed the uncertainty propagation of a multiscale poromechanics-hydration model for concrete by means of stochastic meta-models using polynomial chaos expansions (Venkovic et al., 2013). The sensitivity indices of the input parameters have been computed which revealed the dominant role of the apparent activation energy of calcium aluminate and the elastic modulus of low density calcium-silicate-hydrates (C-S-H) phase for the percolation threshold as well as the poroelastic properties in early-age stages at the cement paste scale. Berveiller et al. have discussed the influence of uncertain input parameters on the variability of the Young's modulus and the Poisson's ratio of cement paste (Berveiller et al., 2009). By means of a multiscale sensitivity analysis based on polynomial chaos expansions, the importance of the volume fraction of high-density C-S-H has been reported.

However, a detailed study on the propagation of uncertainties across the length scales of concrete has not been made yet. The present paper aims to determine the influence of stochastic uncertain input parameters on the model responses of a multiscale elastic analysis quantitatively. Particularly, the Young's modulus of cement-based materials, covering cement pastes, mortars and concretes made of ordinary Portland cement for different water-to-cement ratios at varying hydration stages, is investigated. A framework for a comprehensive probabilistic model assessment methodology applied to a multiscale model based on continuum micromechanics is proposed. The total-effect sensitivity indices in the context of a global, variance-based sensitivity analysis are computed. Moreover, an uncertainty analysis comprising studies on the parameter uncertainty, the model uncertainty, and the total uncertainty is performed in order to compare the stochastic model responses of two different hydration models in the multiscale modeling. In this paper, two commonly utilized hydration models are employed to determine phase volume fractions: the Powers-Acker hydration model (Powers and Brownyard, 1948; Acker, 2001) and the hydration model proposed by Bernard (Bernard et al., 2003) and refined by Pichler et al. (2007).

The paper is organized as follows. In Section 2, the fundamentals of continuum micromechanics are recalled and the deterministic multiscale model for concrete is described. In Section 3, the probabilistic multiscale modeling is performed considering uncertainties in all input parameters. The sensitivity indices as well as the uncertainties of the model predictions at different stages of the hydration process are presented in Section 4. The paper finishes with concluding remarks and future recommendations.

2. Deterministic micromechanical model

Theoretical fundamentals of micromechanics as well as of modeling and homogenization methods implemented in this study have been reported by (Hershey, 1954; Eshelby, 1957; Hill, 1963; Kröner, 1977; Zaoui, 2002; Dormieux et al., 2006). Subsequent investigations by (Bernard et al., 2003; Constantinides and Ulm, 2004; Sanahuja et al., 2007; Pichler et al., 2008; Smilauer and Bittnar, 2006; Shahidi et al., 2014) extended the principles towards the application to cement-based materials, particularly the upscaling of elastic, strength, and creep properties. The continuum micromechanics-based models take into account intrinsic elastic properties of the constituents, the evolution of volume fractions during the hydration process, interactions between phases, and the shapes of the phases.

2.1. Micromechanical representation of concrete

Within the framework of continuum micromechanics, the concept of representative volume elements (RVE) including the scale separation requirement is followed (Drugan and Willis, 1996). The microstructure of concrete cannot be resolved and described in every detail. Thus, at each length scale, a RVE consisting of quasi-homogeneous subdomains with known physical quantities is defined (Pichler and Hellmich, 2011).

The morphological model of concrete is adopted from (Pichler et al., 2007). The model comprises four length scales which are shown in Fig. 1. For the sake of simplicity, the shapes of all embedded phases are assumed to be sphericular, albeit it has been reported that the accuracy of the model predictions increases with consideration of different phase morphologies (Sanahuja et al., 2007; Pichler et al., 2008). The lowest scale, the *nanoscale*, comprises inclusions of high-density C-S-H (CSH-HD) embedded in a matrix of low-density C-S-H (CSH-LD), the air and the water phase, and the four clinker phases. The nomenclature of the two types of C-S-H is taken from Jennings (2000), who distinguishes the phases according to the hydration process. In a matrix of homogenized C-S-H phases, water and air inclusions are embedded (porous C-S-H).

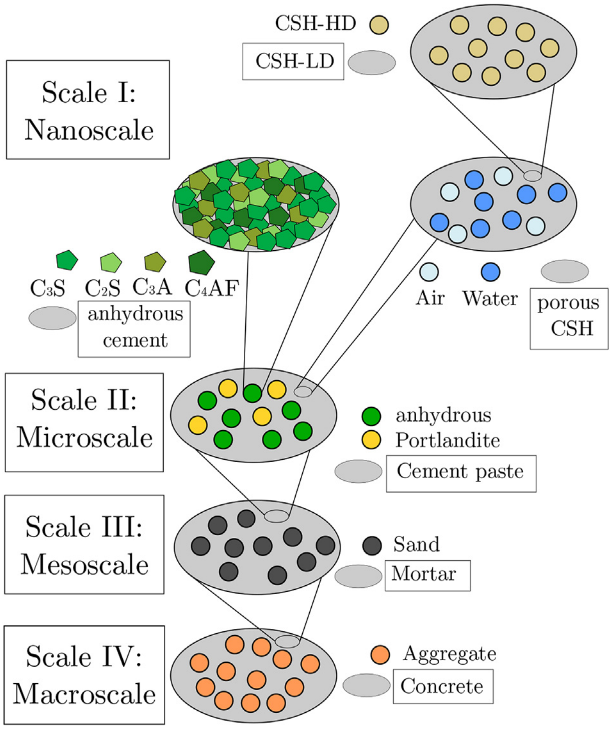

Fig. 1. Scales of observation of the continuum micromechanics-based multiscale model for concrete comprising four length scales (adapted from (Pichler et al., 2007)). Two-dimensional sketches of three-dimensional structures are presented.