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Study of methods for simulating multiphase construction materials

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Abstract

Computer-aided design and multiscale modeling and analysis can lead not only to a better understanding of the behavior of multiphase materials or increased performance, but also reduced energy consumption and raw materials, optimization and cost reduction. Generally, concept modeling involves multiscale analysis, which occurs at two or more levels, from the smallest scale (micro- or even nano-structure) to full system level (macroscopic scale). The purpose of this paper is to analyze the simulation feasibility of multiphase materials (traditional mortar), and also the comparison methods that can be applied in this regard.

This paper introduces a multiscale modeling approach to simulate the effective (macroscopic) mechanical properties of the ordinary cement-based mortar. Simulations of multiphase materials have been done by mean-field homogenization techniques and the finite element method. Multiscale modeling helps to evaluate the stress–strain behavior and reveals important engineering properties, such as Young's Modulus and Poisson's ratio.

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1. Introduction

Theories on understanding and predicting the behavior of multiphase materials is not a new development, numerous theories were developed and improved over the time, starting with the various homogenization methods (e.g. Hill, Voigt, Reuss, Eshelby, Mori-Tanaka) as well as numerical methods. In recent years, due to the fast development of computing technologies, a large variety of physical and engineering problems have been solved

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through the use of numerical techniques. In the field of computer-aided engineering and materials technology, the latest trend is combining micromechanical theory with numerical methods. This kind of approach helps engineers study the behavior of various materials with different kind of constituents, which help reduce development costs and time, facilitating a better understanding and resulting in innovative and high-quality materials [1][2].

This paper presents and examines two prediction methods for analyzing heterogeneous materials. One such method is computer homogenization, based on the nonlinear semi-analytical homogenization theory, and the finite element method, which has been used since the 1970s in several engineering applications. Both methods in this study assume multi-scale material modeling, namely solving the problems at multiple scales (e.g. macro-, micro- or mesoscale).

This paper highlights the Mori-Tanaka Approximation implemented in the Digimat software and used for material modeling, using which the link between the two-scale modeling levels can be determined: the macro- and the meso-scale. At macroscale the mortar can be viewed as a homogeneous material, while at meso-scale it can be considered a composite made up of a cement paste matrix with fine aggregate embedded in it and pores (air voids). The interfacial zone between the inclusions and the matrix can be a constituent, too.

Since a significant part of the volume of mortars is occupied by fine aggregate, its quality and properties have considerable importance in the composite's properties, consequently affecting the durability and structural performance of mortars. The aggregate is not only cheaper than cement, but also has a higher volume stability and better durability than hydrated cement paste alone. In this study, fine aggregate was viewed as a dispersed material throughout the cement paste, and experimental and virtual tests were conducted in this regard.

2. Theoretical background of the computer modeling and simulation of homogeneous materials

Any homogeneous and isotropic material can be represented at a certain scale as a composite made up of a finite or infinite number of constituent elements or sub-elements. The behavior of these composite materials or multiphase materials in general is difficult to be defined due to their microstructure, so modeling and analyzing it presents a challenge in materials engineering. In order to simulate the behavior of a multiphase material, multi-scale modeling can be used, taking into account the interaction of the constituent phases and its properties. At present, virtual mechanical testing of heterogeneous materials is carried out at the micro level up to the macro level, depending on the precision required. Multiscale modeling helps us evaluate the stress-strain behavior and reveals important engineering properties, such as Young's Modulus and Poisson's ratio. The objective of this type of modeling is to predict the interaction between the macroscopic (effective) properties and the scale below it (meso- or in some cases microscopic properties). The different levels can be linked by averaging methods, i.e. using homogenization techniques through a Representative Volume Element (RVE) concept. To do this, we must know the properties of the different phases that can be considered individually heterogeneous (physical parameters, global/effective or macro-level material constants), the distribution and shape of the inclusions in the matrix. [2][4][5]

Based on the mean field theory, homogenization represents the determination of macroscopic or effective properties of the heterogeneous materials, based on the analysis of RVE, and calculated as the averages of the corresponding micro fields. RVE is the representation of a small sample cut from the material, an idealization of the meso- or microstructure of the heterogeneous material. Using this method, it is assumed that the macroscopic/effective properties are equal to the average mechanical properties of an RVE. In terms of stresses and strains, the concept of homogenization can be formulated by:

$$\bar{\sigma} = \langle \sigma \rangle_{\omega} = \frac{1}{V} \int_{\omega} \sigma dV; \quad \bar{\varepsilon} = \langle \varepsilon \rangle_{\omega} = \frac{1}{V} \int_{\omega} \varepsilon dV \quad (1)$$

where $\langle \rangle$ denote the average of the stress/strain field over the RVE (domain ω and volume V).

Equations (1) do not solve the problem of homogenization, namely the equivalence of the inhomogeneous volume with a homogeneous one, which takes into account the properties of the constituent phases. In order to establish the relationship between the constituent phases, the concentration tensor has been introduced. This can be written in mathematical terms according to stresses and deformations as follows:

$$\langle \sigma \rangle_{\omega_k} = A_k \langle \sigma \rangle_{\omega}; \quad \langle \varepsilon \rangle_{\omega_k} = B_k \langle \varepsilon \rangle_{\omega} \quad (2)$$

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