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Digital image based numerical micromechanics of geocomposites with application to chemical grouting

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ABSTRACT

The presented paper describes procedures of numerical upscaling and experience with X-ray CT based finite element (FEM) analysis of properties of geocomposites. The upscaling technique is used for obtaining the macro-level response of material by loading test (representative) volumes with described micro-level structure. The application is focused on geocomposites arising from chemical grouting of coal substances. The obtained (homogenized) macro-level properties serve for solving stability problems by numerical modeling in geotechnical engineering. The paper touches several interacting topics – numerical upscaling and understanding to its results; application of X-ray computed tomography (CT) for visualization of structure of geomaterials; processing the digital image data for constructing FEM models of test volumes; numerical testing of digitalized samples for obtaining homogenized properties and clearing up sensitivity to changes in local material properties, micro-level structure and FE mesh; validation of numerical results by comparison with laboratory testing of samples; use of identification technique for refining the local material properties and calibration of the upscaling procedure.

1. Introduction

In geotechnics, one uses a variety of technological procedures for modification of rock or soil properties for different purposes like decreasing permeability for remediation, reinforcement for building of surface and underground constructions, stabilization of openings for mining etc. These modifications can use piles, anchors and also various grouting procedures with cementitous or polymer based (chemical) grouts [1,2]. As a result, the natural geomaterials are modified into geocomposites with properties more suitable for engineering purposes.

Chemical grouting is also used in coal mining for strata stabilization [3,4] and especially coal seam grouting provides motivation for investigation of coal-resin geocomposites [5]. This investigation aims in answering questions how the mechanical behavior of geocomposite is influenced by the original coal structure, filling of fractures and voids, properties of the polyurethane resin etc. The methodology of investigation is based on testing samples of coal geocomposites, which are developed in the laboratory [5]. This methodology uses laboratory testing of deformation and strength properties, but also visualization of inner structure of geocomposites and structural changes under loading. This paper shows that X-ray CT visualization of the microstructure can be amended by numerical simulations of the loading tests by using finite element models constructed from digital images and local material properties.

In the numerical simulations, the geocomposites are considered to be two-scale materials. The macro-scale corresponds to the role of geocomposite in engineering constructions and its characteristics length $L > 100$ mm. This length also corresponds to the size of (the smallest) finite elements used for analysis of geoengineering problems. The micro-scale lengths are 100 or more times smaller, to represent the fractures and voids filled with polyurethane resin in different levels of foaming. We use micromechanics to analyze and clarify the dependence of the macro-scale behavior on the micro-scale, i.e. the influence of micro-level structure geometry and local material properties. We can call this process as upscaling and a short description of the exploited procedures will be presented in Section 2. Here, we shall discuss numerical testing with different forms of the applied boundary conditions and touch some questions of anisotropy of the macro-scale response. Besides the testing the linear elastic behavior, we only mention the testing of the inelastic material behavior. The described mathematical procedure will be applied to the analysis of coal geocomposites, which are more thoroughly described in Section 3.

Tensors. In the sequel we consider vectors $v \in R^3$ with components v_i $(i = 1, 2, 3)$, symmetric second order tensors $\xi \in \mathrm{T}(3, 2)$ with components ξ_{ij} $(i, j = 1, 2, 3)$ and symmetric fourth order tensors $X \in \mathrm{T}(3, 4)$ with components X_{ijkl} $(i, j, k, l = 1, 2, 3)$, $X_{ijkl} = X_{jikl} = X_{ijlk}$

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$=X_{klij}$. We use scalar products and corresponding norms

$$u\cdot v=\sum_i u_i\,v_i,\quad \xi:\eta=\sum_{ij}\xi_{ij}\,\eta_{ij},\quad X:Y=\sum_{ijkl}X_{ijkl}\,Y_{ijkl},\quad \|u\| =\sqrt{u\cdot u},\quad \|\xi\|=\sqrt{\xi:\xi},\quad \|X\|=\sqrt{X:X}\,.$$

For symmetric positive definite tensors X, Y the inequality $X\le Y$ means that $\xi:(Y-X):\xi\ge 0$ for all $\xi\in \mathrm{T}(3,2)$. We shall also use identity $I\in \mathrm{T}(3,4)$, $I\xi=\xi$ for all $\xi\in \mathrm{T}(3,2)$, $(I)_{ijkl}=\frac{1}{2}(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})$, where δ is the Kronecker's delta. Any $\xi\in \mathrm{T}(3,2)$ can be uniquely decomposed into volumetric and deviatoric parts, $\xi=\xi_{vol}+\xi_{dev}$, $\xi_{vol}=I_V:\xi$, $\xi_{dev}=I_D:\xi$, $(I_V)_{ijkl}=\frac{1}{3}\delta_{ij}\delta_{kl}$, $\|I_V\|=1$, $I_D=I-I_V$, $\|I_D\|=\sqrt{5}$, $I_V:I_D=I_D:I_V=0$.

2. Numerical upscaling

The procedure for investigation of influence of micro-level structure to macro-level material properties starts with definition of the test volume (TEV) Ω as a macro-level size sample of the material involving micro-level structure. The test volume TEV is equal to representative elementary volume (REV) standardly used in the homogenization theory if it provides unique complete information about the macro-level material properties. If it is smaller due to restricted knowledge, it can still provide useful information. Let us assume that Ω is given with information about the microstructure (geometry and local material properties). Then the test volume is loaded on the boundary, to get its mechanical response and obtain the macro-scale characterization. Note that the micromechanics usually works with representative volumes, which provide some statistically homogeneous information, our test volumes can provide weaker, but still useful information about the macro-level material behavior. First, we assume linear elastic material behavior, which is given by elastic behavior of the constituents and no occurrence of debonding between the constituents (material phases). The deformation of Ω under the loading is described by the boundary value problem

$$div(\sigma)=0,\quad \sigma=c:\varepsilon,\quad \varepsilon=\frac{1}{2}(\nabla u+\nabla u^T)\ \text{ in }\Omega \quad +\text{boundary conditions on }\partial\Omega. \tag{1}$$

where $\sigma=\sigma(x)$, $\varepsilon=\varepsilon(x)$, $C=C(x)$ are stress, strain and elasticity tensors, respectively. As the volume forces are considered to be zero, the loading is imposed via the boundary conditions exclusively.

We can consider different types of boundary conditions, which will influence the testing. Let us consider the following possibilities:

$$u(x)=\ \xi_\varepsilon\cdot x\ \text{ on }\partial\Omega,\ \text{where } \xi_\varepsilon \text{ is a prescribed symmetric second order tensor,} \tag{2}$$

$$\sigma(x)\cdot n(x)=\xi_\sigma\cdot n(x)\ \text{ on }\partial\Omega,\ \text{ where } \xi_\sigma \text{ is again a prescribed tensor,} \tag{3}$$

$$\text{mixed Dirichlet}-\text{Neumann BC on }\Gamma_0,\Gamma_1,\ \text{where }\Gamma_0\cup\Gamma_1=\partial\Omega,\ \Gamma_0\cap\Gamma_1=\varphi, \tag{4}$$

$$\text{periodic boundary conditions.} \tag{5}$$

where Ω is TEV of arbitrary shape for BC (2) and (3). Moreover, we assume that Ω is a cuboid or cylinder for BC (4) and cuboid for BC (5). The unit outer normal to the boundary $\partial\Omega$ is denoted by n.

On the macro-scale, we consider the test volume Ω as a homogeneous body with (homogenized) material properties given by the elasticity tensor $\overline{C}$, which defines relation between macro-stress $\overline{\sigma}$ and macro-strain $\overline{\varepsilon}$. If standard averaging provides the relation between micro and macro stresses and strains, then

$$\overline{\sigma}=\langle\sigma\rangle=|\Omega|^{-1}\int_\Omega\sigma(x)\,dx,\ \overline{\varepsilon}=\langle\varepsilon\rangle=|\Omega|^{-1}\int_\Omega\varepsilon(x)\,dx,\quad |\Omega|=\int_\Omega dx \tag{6}$$

and the elasticity tensor $\overline{C}$ or its inverse $\overline{C}^{-1}=\overline{D}$ can be determined from the stress-strain relations

$$\overline{\sigma}^{(k)}=\overline{C}\,\overline{\varepsilon}^{(k)}\ \text{ or } \overline{\varepsilon}^{(k)}=\overline{D}\,\overline{\sigma}^{(k)} \tag{7}$$

where $\overline{\sigma}^{(k)}$, $\overline{\varepsilon}^{(k)}$ are pairs of averaged stress and strain, the upper index indicates that this stress and strain corresponds to k-th case of loading, which corresponds to application of different boundary conditions. For example $\overline{\sigma}^{(k)}$, $\overline{\varepsilon}^{(k)}$ can be computed from testing with boundary conditions (2) or (3) with $\xi_\varepsilon=\xi^{(k)}$ or $\xi_\sigma=\xi^{(k)}$, $k=1,\dots,6$, where

$$\xi^{(1)},\dots,\xi^{(6)}=\begin{bmatrix}1&0&0\\0&0&0\\0&0&0\end{bmatrix},\ \begin{bmatrix}0&0&0\\0&1&0\\0&0&0\end{bmatrix},\ \begin{bmatrix}0&0&0\\0&0&0\\0&0&1\end{bmatrix},\ \times\begin{bmatrix}0&1&0\\1&0&0\\0&0&0\end{bmatrix},\ \begin{bmatrix}0&0&1\\0&0&0\\1&0&0\end{bmatrix},\ \begin{bmatrix}0&0&0\\0&0&1\\0&1&0\end{bmatrix}. \tag{8}$$

The use of boundary conditions (2) guarantees that $\overline{\varepsilon}=\xi_\varepsilon$, and similarly the use of Eq. (3) provides $\overline{\sigma}=\xi_\sigma$ [6]. It provides a direct possibility of computation of $\overline{C}$ from

$$\left\langle\sigma^{(k)}\right\rangle=\overline{C}:\xi^{(k)},\quad k=1,\dots,6 \tag{9}$$

or $\overline{D}=\overline{C}^{-1}$ from

$$\left\langle\varepsilon^{(k)}\right\rangle=\overline{D}:\xi^{(k)},\quad k=1,\dots,6. \tag{10}$$

Note that it is advisable to symmetrize the computed tensors $\overline{C}$, $\overline{D}$ to get all required symmetries exactly. The Hill condition is fulfilled for all cases (2)–(5). If $\overline{C}_\varepsilon$ is computed from Eqs. (1), (2), (9) and if $\overline{D}_\sigma$ is computed from Eqs. (1), (3), (10) then the following bounds

$$\overline{D}\le\overline{C}_\sigma\ \le\ \overline{C}_\varepsilon\le\ \overline{C}_\varepsilon \tag{11}$$

are valid with inequalities among tensors in the energetic sense, see Introduction. $\overline{C}_\varepsilon=\langle C(x)\rangle$ denotes the Voight and $\overline{D}_\sigma^{-1}=\left\langle C^{-1}(x)\right\rangle$ provides the Reuss estimate ($\langle C(x)\rangle$ denotes again averaging over the domain Ω). For more details see [6–11].

The homogenized tensor also depends on the size of the test volume Ω and in the ideal homogeneous case all tests with different boundary conditions provide the same elasticity tensor. In a non ideal case, the difference

$$\max\left\{\xi\in\mathrm{T}(3,2),\ \sqrt{\xi:(\overline{C}_\varepsilon-\overline{D}_\sigma^{-1}):\xi}\right\}\le\|\overline{C}_\varepsilon-\overline{C}_\sigma\| \tag{12}$$

can serve as a measure of macro-scale homogeneity and proper size of Ω.

In the case of coal geocomposites, the upscaled elasticity tensor obtained by numerical testing possesses general anisotropy, but frequently we do not expect that some apparent anisotropy should be presented in our macro-scale problem (it may not be the case in another applications). Therefore, we can seek for isotropic elastic tensor $\overline{C}_{iso}$, which will approximate well the anisotropic tensor $\overline{C}$. Note that similar problems of approximation appear also in crystallography and seismology. Due to the simple representation of the isotropic elasticity tensors

$$\overline{C}_{iso}=3K\,I_V+2G\,I_D, \tag{13}$$

where I_V and I_D, which serve for decomposition into volumetric and deviatoric component are defined in Introduction. Using derivation and orthogonality of I_V and I_D, it can be easily seen that the best approximation $\|\overline{C}_{iso}-\overline{C}\|=\min_{K,G}$ is obtained for K, G