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On the effective transport properties of heterogeneous materials

Sy-Tuan Nguyen[a,b,*], Duc-Chinh Pham[c], Minh-Ngoc Vu[b], Quy-Dong To[b,d]

[a] Euro-Engineering, 4 rue Jules Ferry, 64000 Pau, France
[b] Duy Tan University, Institute of Research & Development, K7/25 Quang Trung, Danang, Vietnam
[c] Institute of Mechanics-VAST, 264 Doi Can, Ba Dinh, Hanoi, Vietnam
[d] Laboratoire Modelisation et Simulation Multi Echelle, MSME UMR 8208 CNRS, Universite Paris-Est, 5 Boulevard Descartes, 77454 Marne-la-Vallee Cedex 2, France

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ABSTRACT

This paper provides a new homogenization scheme, which is a combination of the theoretical and experimental approaches, for modeling effective transport properties of heterogeneous materials. Differ from the classical methods, this method considers a free conductivity of the reference matrix that is not a pre-defined parameter and can be calibrated based on an inverse analysis using available microscopic and macroscopic data. This technique is illustrated using experimental data of electrical conductivity of rocks published in literature. We show that the conductivity of the reference matrix can be approximated by linear or quadratic functions of the porosity. The proposed approach can be used to model materials containing highly contrast phases.

1. Introduction

Transport properties of materials (permeability, thermal conductivity, electrical conductivity and diffusivity) are very important properties required for many industrial studies. For example, permeability is needed for the prediction of oil and gas productivity (Raghavan & Chin, 2002). Thermal conductivity is necessary for simulations of geothermal production (Barbier, 2002; Jaeger, 1965) or for the design of civil engineering structures subjected to thermal loading (e.g. waste storage, coke ovens, furnaces). The processing of electrical resistivity is an effective technique to predict porosity, mineralogical compositions, pore pressure and in-situ stress in sediment basins (Eaton, 1975). Electrical resistivity can be also used to follow the hydration of cement at early age (Backe et al., 2001). Finally, diffusivity is an important property required to analyze the damage of civil materials due to chemical attacks (corrosion, erosion) (Tixier & Mobasher, 2003).

Transport properties of a material can be directly measured in laboratory. However it is impossible to use the experimental approach to deal with the variety of the materials' composition and microstructure (e.g., shape, distribution and connection of the phases). The basic idea to overcome this problem is to use empirical methods that consist to interpolate and extrapolate experimental data by simple mathematical laws (Archie, 1942; Mavko & Nur, 1997). However, these empirical laws require many measurements that demand sometime enormous time and budget. For example, measurement of permeability of a low permeable rock such as clay stone require several months. Besides, it is not evident to take a sample in a deeply rock formation and to protect it in field condition when bring it to laboratory.

* Corresponding author at: Res. Les Chenes 2, N° 5 rue Pasteur Alphonse Cadier, 64000, Pau, France.
E-mail address: stuan.nguyen@gmail.com (S.-T. Nguyen).

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Thus, numerical and analytical approaches are considered together with experimental method to study effective transport properties of natural and man-made materials. The finite element method (FEM) allows simulating the "real" microstructure of materials (Vignal et al., 2002) that can be captured by 3D images. Such simulations are usually very costly due to the microstructure's complexity. For example concrete or clayey rocks are highly heterogeneous materials from nano scale to micro scale (Ulm et al., 2004). Accordingly, it is impossible to use FEM for such microstructure. Most importantly, microcracks and imperfect interfaces between the local phases strongly affect the transport properties of the whole domain but they cannot be identified by 3D images.

For many decades, homogenization approaches such as Maxwell, self-consistent, Mori–Tanaka, differential effective medium, Hashin–Shtrikman bounds are usually used to predict effective mechanical and transport properties of heterogeneous materials (Hashin & Shtrikman, 1963; Maxwell, 1904; Mori & Tanaka, 1973; Nguyen et al., 2015a, 2015b, 2015c; O'Connell & Budiansky, 1974; Pham, 2000; Pham & Nguyen, 2015). The main idea of these approaches is to relate the local response of the inhomogeneities to the macroscopic boundary condition applied on a Representative Elementary Volume (REV) (Dormieux et al., 2006; Eshelby, 1957; Nguyen, 2014a). The complex microstructure of a real material is simplified to an equivalent simple microstructure. For example the spherical shape is usually assumed for a quartz grain (Nguyen et al., 2015b) and the penny-shape is usually considered for a crack (Nguyen et al., 2011; Pouya & Vu, 2012; Vu et al., 2015). The orientation and spatial distribution of the phases can be also considered (Castañeda & Willis, 1995). For materials that exhibit the heterogeneity at many scales, multi-scale homogenization technique can be considered (Bernard et al., 2003; Nguyen et al., 2015c; Ulm et al., 2004). Due to these features, analytical homogenization method is suitable for predicting effective mechanical and transport properties of any kind of materials. For example, Nguyen and colleagues developed analytical solutions for effective electrical conductivity and anisotropy of rocks (Nguyen, 2014a; Nguyen et al., 2015a) and effective viscoelastic properties of cracked materials (Nguyen, 2014b; Nguyen et al., 2011).

In practice, each homogenization scheme is applicable for a particular medium. For example, Mori–Tanaka scheme can be used for materials with a major connected matrix (ex. concrete can be considered at micro to meso scales as a mixture of cement matrix and grains) while self-consistent scheme can be used for perfect disordered materials (e.g. polycrystals). However, choosing an appropriate scheme for a case is sometime difficult due to the lack of microscopic information.

To deal with those difficulties, Pham and Nguyen (2015) propose a polarization method for thermal conductivity of composites. The idea is to keep the conductivity of the reference matrix as a free parameter that is calibrated using a single experimental point. Basically, changing this free parameter allows passing from one homogenization scheme to another. Indeed, this free parameter equals to the minimum or maximum conductivities of the phases of the mixture yields the lower and upper Hashin–Shtrikman bounds. This parameter equals to zero or infinity corresponds to the Voigt–Reuss bounds. A free parameter equal to the conductivity of the major connected phase or the overall conductivity of the mixture is equivalent to the Mori–Tanaka scheme or the self-consistent one, respectively. The results obtained from the polarization method lay on one measure point and close to the other points.

To optimize the polarization method proposed previously by Pham and Nguyen (2015), this paper provides a new homogenization scheme, which is a combination of the theoretical and experimental approaches, that considers a free conductivity of the reference matrix that can be calibrated based on an inverse analysis using all available experimental data. Firstly the theoretical basis of the homogenization approaches is reviewed. A flexible adaptive Eshelbian homogenization scheme is then developed. Finally, an application for electrical conductivity of rocks using experimental data published in literature is considered.

2. The theoretical basis of the homogenization approach

The overall conductivity of a heterogeneous medium can be obtained by considering the relationships between the local and the macroscopic behaviors of a REV (the size of REV must be very large comparing with the local size of the inhomogeneities and must be very small comparing with that of the medium) that are resumed by the following equations (Dormieux et al., 2006):

$$\underline{\sigma}(\underline{z}) = -\boldsymbol{c}(\underline{z}).\underline{e}(\underline{z}) \tag{1}$$

$$\underline{\Sigma} = -\boldsymbol{C}^{hom}.\underline{E} \tag{2}$$

$$\underline{\Sigma} = \frac{1}{|\Omega|}\int_{\Omega}\underline{\sigma}(\underline{z})d\Omega \tag{3}$$

$$\underline{E} = \frac{1}{|\Omega|}\int_{\Omega}\underline{e}(\underline{z})d\Omega \tag{4}$$

where $\underline{\sigma}(\underline{z})$, $\underline{e}(\underline{z})$ and $\boldsymbol{c}(\underline{z})$ are the local flux vector, gradient field and conductivity tensor at a point $\underline{z}$ inside the REV, respectively; $\underline{\Sigma}$, $\underline{E}$ and $\boldsymbol{C}^{hom}$ the overall flux vector, gradient field and conductivity tensor of the REV; Ω is the REV and $|\Omega|$ its volume. The local and average gradient field tensors are related by the following linear equation (Eshelby, 1957):

$$\underline{e}(\underline{z}) = \boldsymbol{A}(\underline{z})\underline{E} \tag{5}$$