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Equivalent microstructure problem: Mathematical formulation and numerical solution

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ABSTRACT

Analytical homogenization schemes, including the Mori–Tanaka (M–T) or Self-Consistent (S-C) schemes, are computationally attractive tools for estimating the homogenized properties of porous media. Utilizing these approaches, we evaluate the effective properties based on the solution of single inclusion problem and assuming a simplified morphology of microstructure (usually a finite number of inclusion families is postulated). The simplified microstructure is the main disadvantage of these methods since it does not conform in a geometrical sense to the microstructure of a real porous medium. In this work, we formulate the inverse problem of micromechanics in which we aim to identify a so-called equivalent microstructure for the real porous material. This microstructure has to preserve the overall response (thermal conductivity) that is analogous to that of real porous material, regardless of the conductivity of the fluid occupying the pore space. The equivalent microstructure (still simplified with respect to the real one) is a virtual one with morphology of oblate spheroids (pore space) embedded in a solid matrix (skeleton). The distribution of inclusions is described by the probability density function with a random variable being the semi-axis aspect ratio θ. The inverse problem is formulated as a linear Fredholm equation of the first kind supplemented with additional constraints. Stochastic optimization procedure is used to solve the inverse problem, i.e. identification of the probability density function. The methodology is verified against the theoretical results obtained via classical bounds on the effective thermal conductivity. Finally, the procedure is applied to real porous material, and an equivalent microstructure for sand, with respect to the overall thermal conductivity, is identified.

1. Introduction

Porous media are highly heterogeneous materials composed of a skeleton (solid phase, usually referred to as the matrix) and pore space that is occupied by a gas and/or liquid. Typical examples of naturally porous materials are porous rocks and soils. Such materials have been a subject of extensive research and analyses for many years due to their properties related to heat transport (insulators), filtering of various media, storage of gases and vapours, etc. (Bussian, 1983; Dye, McClure, Gray, & Miller, 2015; Glover, Hole, & Pous, 2000; Ordonez-Miranda & Alvarado-Gil, 2012). In recent decades, special attention has been given to the up-scaling of structural properties of porous media from the micro-scale to that of engineering applications. At the scale of the heterogeneities, the properties corresponding to particular constituents or phases

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are usually denoted as micro-properties, whereas at the engineering application scale the properties are usually referred to as the macro, overall, effective or homogenized properties. The techniques used for estimating the overall properties of micro-heterogeneous media, based on the phase properties and microstructure morphology, are referred to as continuous micromechanics (Dormieux & Ulm, 2005; Dormieux, Kondo, & Ulm, 2006; Li & Wang, 2008; Mura, 1987; Suquet, 1997). In general, there are two, methodologically different approaches: analytical approximation schemes (discussed, e.g., in Christiensen, 1990; Hashin, 1983; Hill, 1965; Kachanov, 1992; Mori & Tanaka, 1973; Sevostianov & Kachanov, 2014) and computational micromechanics (e.g., Kanit, Forest, Galliet, Mounoury, & Jeulin, 2003; Zohdi & Wriggers, 2008). Analytical approximation schemes such as the Self-Consistent (S-C) scheme, Mori–Tanaka (M–T) approach, Maxwell approach or Differential Effective Medium approach, as well as their subsequent modifications, are based in general on the solution of a single ellipsoidal inclusion embedded in an infinite and continuous medium. The attractiveness of analytical approaches are due to their mathematical simplicity, which is a direct consequence of the simplifications within the modelling of the interactions between inclusions, as well as, due to the assumption of a "primitive" (in relation to the real porous microstructure) morphology of the microstructure, such as penny shaped cracks, spherical and spheroidal or superspherical inclusions immersed in a continuous matrix (Hill, 1965; Mori & Tanaka, 1973; Sevostianov & Giraud, 2013; Torquato, 2002). However, this simple microstructure which results in the attractiveness of analytical approximation schemes, is on the other hand, their main disadvantage – the microstructure morphology, where the pore space is created from a set of ellipsoidal inclusions, does not conform in a geometrical sense to the microstructure of a real porous medium.

Recently, advanced laboratory techniques, including X-ray microCT, have enabled the 3D reconstruction of material microstructures (Schwartz et al., 1994). Due to the random nature of porous materials (which is revealed in the grains/pores orientations, shapes and its spatial distribution)) their microstructures are usually very complex (Kaviany, 2012; Torquato, 2002). Therefore, for macroscopic properties evaluations, a computational micromechanics is very often utilized (Sab, 1992; Zohdi and Wriggers, 2008). Within this approach, the homogenized properties are usually sampled via the Monte Carlo simulations (Dalaq, Ranganathan, & Ostoja-Starzewski, 2013; Kanit et al., 2003; Łydżba & Różański, 2014) by considering a finite set of random realizations of the representative volume elements (rve). Generally, except for problems resulting from the use of numerical techniques (e.g., numerical errors, contrast in the mechanical properties of different phases, convergence, etc.), there are two main problems associated with this approach: both the proper size of the rve and a sufficient number of realizations must be evaluated. Some details on these issues are provided, e.g., in the work of Łydżba and Różański (2014). Computational micromechanics calculations, regardless of the numerical technique that is used, are usually time consuming, meaning that the application of this approach to digital representations of porous media for the purposes of effective properties evaluations results in a large computational effort (Kanit et al., 2006).

The problems indicated for computational micromechanics show that analytical homogenization schemes can be still computationally attractive tools to estimate the homogenized properties of porous media, provided that any porous medium can be associated with a virtual, simplified microstructure whose overall response is analogical to the real porous material. In this paper we focus on macroscopically isotropic porous media. We propose a technique to identify such a simplified morphology with respect to a heat conduction problem. The morphology of virtual microstructure is assumed to be of a matrix/inclusion type with oblate spheroids (pore space) embedded in a solid matrix (skeleton). The infinite number of spheroidal inclusion families is, however, postulated. The distribution of inclusions is characterized by the probability density function with a random variable being the semi-axis aspect ratio θ. The virtual microstructure is imposed to be invariant with respect to fluid thermal conductivity which means that it has to imply the same overall response as the original/real medium for an arbitrary fluid occupying the pore space; then, the simplified microstructure will be referred to as the equivalent microstructure. For this purpose, we formulate an appropriate inverse problem that we propose to solve using a stochastic optimization approach. The methodology is verified against theoretical results obtained with classical bounds on the effective thermal conductivity. Finally, the method is applied to a real porous material (medium sand), and the equivalent microstructure is identified. We note here that we are considering a conductive heat flow problem, but the proposed technique can be successfully applied to different problems with the same mathematical structure, including the electrical conductivity, diffusion, etc.

The paper is organized as follows. In next section, the concept of the overall microstructure response function is formulated. Next, the integral equation, being a basis of identification procedure for an equivalent microstructure, is derived. In Section 4, the stochastic optimization procedure, used for the numerical solution of the inverse problem, is formulated. Section 5 describes the verification procedure and presents the results from these preliminary computations. Next, the microstructure and physical properties (density, porosity, particle size distribution, etc.) of the real porous material, the medium sand, are provided. For this material the results from laboratory measurements for the overall thermal conductivities are also given. The equivalent microstructure for the material considered is then identified. Finally, Section 7 presents our conclusions.

2. Overall microstructure response function

We consider the porous medium of a volume V composed of a homogeneous solid skeleton (occupying the volume V_s) and pore space occupying the volume V_f filled with some fluid (a liquid or gas). The steady-state heat conduction process,