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Research Paper

A comparison of discrete element and micromechanical methods for determining the effective elastic properties of geomaterials

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ABSTRACT

Data generated from scanning electron microscopy images of oil-shale geomaterials are used to generate configurations and to acquire parameters required for use in homogenization schemes for the determination of the effective elastic properties of the samples. Two alternative homogenization methods are employed: numerical simulation using the Discrete Element Method and the Polycrystalline Self-Consistent Method from micromechanics. The schemes give rise to predictions of the effective elastic properties that are in very good agreement.

1. Introduction

Geomaterials possess all manner of heterogeneity at a number of lengthscales. Estimating the mechanical properties of such media has therefore attracted a great deal of attention over the years, e.g. [1]. On the large scale, one can visually detect heterogeneities and discontinuities, i.e. bedding planes, faults, pores and cracks for example. Similarly, inhomogeneity is present at the microscale, although often not detectable by the human eye. Such microscale inhomogeneities include those types mentioned at the larger scale but also micropores, microcracks, mineral grains and crystals, to name but a few. These inhomogeneities will in general induce strong anisotropy in the material. A common approach is to attempt to define a so-called *representative volume element* (RVE) containing a large number of microscale inhomogeneities, distributed in a statistically homogeneous manner. This enables effective, homogeneous, anisotropic properties to be defined associated with the RVE or sample, in question [2,3]. This so-called *homogenization* process is particularly useful when loading conditions are such that fields induced in the sample vary on a length scale much larger than any inhomogeneity length scale. It is also important to note that homogenization can be applied at a so-called *mesoscale* if one wishes, so that large scale heterogeneity can be incorporated into field models if required [4]. Here, two methods are employed in order to estimate the effective homogeneous anisotropic elastic properties of oil-shale geomaterials where the side of the RVE in question is 20 mm: the Discrete Element Method (DEM) and the Polycrystalline Self-Consistent Method (PSCM).

The DEM is used in a wide variety of engineering problems in order to efficiently model discontinuous and continuous media, including problems involving powders and rock mechanics [5,6]. In [7], a two dimensional (2D) DEM was employed in order to estimate the elastic properties of layered geomaterials. DEM systems of approximately 16,000 particles were created, settled, and bonded, and different particle stiffness properties were assigned, based on their location in the DEM system, to represent a petroleum-bearing geomaterial comprised of a mineral and a kerogen component. Effective elastic properties were estimated using the DEM when the sample is subjected to displacement boundary conditions and the medium is approximated as transversely isotropic. Parameter studies were carried out on bonded materials, varying kerogen content, confining pressure, porosity, particle

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resolution, and layer geometry. These studies determined that all parameters, except for confining pressure, have a significant influence on the effective elastic properties of the samples. Chang and Liao [8] establish upper and lower estimates of the elastic moduli for granular materials and relate a micromechanical description of strain to the packing structure. Magnanimo et al. [9] suggests the elastic response of a granular material is dependent on the coordination number, which is linked to the fluctuation of the number of contacts per particle in a granular system subjected to shear strain. Bathurst and Rothenburg [10] developed used microstructure to develop expressions for the elastic constants of granular assemblies with linear contact interactions. Somfai et al. [11] shows that, if a 2D system of particles can be considered a homogeneous 2D material, the macroscopic stress-strain behavior can be described by 4 independent elastic moduli.

Micromechanical methods to predict the effective elastic properties of inhomogeneous media, see for example [3] date back to the pioneering work of [12,13] but the theory was developed significantly in the 1960s due to the associated need to understand composite materials that were being developed at that time. Assuming that an RVE has been identified, standard methods give rise to predictions of the effective elastic properties in terms of so-called *concentration tensors*, linking fields inside certain phases of the medium to the imposed field. Many methods employ techniques associated with the canonical inhomogeneity problem and exploit the useful simplifications that occur for ellipsoidal inhomogeneities giving rise to the useful Eshelby **S**-tensor and Hill **P**-tensor [14]. The simplest such scheme is the so-called *dilute* estimate (DE), based on the seminal work by [15] where interactions between phases are neglected. This method is computationally cheap, explicit, and simple to implement; however, it has been found to have only reasonable accuracy when the volume fraction of inclusion(s) in a host material is small. Extensions to non-dilute volume fractions are numerous but perhaps the most popular include the Mori-Tanaka [16], differential [17], self-consistent [18–21] and generalized self-consistent methods [22]. A variety of self-consistent methods have been proposed. It appears that for geomaterials, the so-called *Polycrystalline self-consistent method* (PSCM) is most appropriate since generally no host medium can be discerned.

Finite element methods have been used in conjunction with Monte Carlo simulations by a number of authors to determine the effect of randomly distributed microstructure on the effective elastic properties of heterogeneous materials. In [23] randomly distributed voids were considered and it was concluded that the predictions were in good agreement with analytic and alternative numerical models. Willoughby et al. [24] and Gusev [25] used similar approaches to obtain estimates of effective properties.

Here, data is acquired from scanning electron microscopy (SEM) images of oil-shale samples in order to generate two dimensional configurations that can be used in the DEM and PSCM. In the case of the DEM a virtual model of a rock sample is created that represents the original rock sample on the microscale both in terms of geometry and mineralogy. Random-pack systems of circular particles are generated in the RVE domain and assigned mineralogical properties based on the SEM data, restricted to six mineral types. Volume fraction data for each of the six mineral phases are also acquired. These particles are then bonded using the parallel bonding algorithm of [5] before the DEM simulations are performed. Two different displacement boundary condition states are then imposed on samples in order to determine the effective elastic properties. For the implementation of the PSCM the standard micromechanical expressions are employed for circular cylinders, for a six-phase medium with volume fractions assigned as those acquired from the images referred to above. Comparisons reveal that both methods give good agreement.

Subscript notation is mainly used in the paper, where the summation convention is implied over repeated indices and the range of the subscripts is 1–3 unless otherwise indicated. In the absence of subscripts, lowercase boldface for vectors (e.g., **a**) is used.

2. Geomaterials and DEM

Oil shale samples provided courtesy of the Center for Oil Shale Technology and Research (COSTAR) at the Colorado School of Mines in Golden, CO, are extracted from the Eocene geologic formation known as the Green River Formation and analyzed using Quantitative Evaluation of Minerals by Scanning Electron Microscopy, or QEMSCAN. More details about this quantitative method can be found in [26]. Details concerning the preparation of the samples prior to QEMSCAN analysis can be found in [27]. Two different QEMSCAN analyses are performed on each of three physical samples. One analysis yielded a two-species representation of the material comprised of pores and solid materials, and the second analysis yielded a multiple-species representation of the sample comprised of various minerals.

2.1. RVE configurations for homogenization derived from imaging

For the DEM-based analyses of the geomaterial data, random pack (RP) systems of particles are generated, settled, and bonded in a square domain. The particles in the 2D systems are assigned mineralogical identities using hashing techniques; this involves converting the geomaterial images into text files using the image processing software *Image J*, discussed in [28]. An example of this conversion is shown in Fig. 1, in which a simple 8-bit, red/green/blue (RGB) 256 by 256 pixel image is converted to a text file; a portion of the text file is displayed in order to show that geometry and color data are preserved during the conversion. Only two different integers identify the colors of the pixels in the black and white image shown on the left side of Fig. 1; a value of 0 represents black, and a value of 255 represents white.

Integrating the information contained in the text files into DEM simulations is achieved by discretizing the domain in which the DEM particles are generated and subsequently settled into a number of regions consistent with the number of pixels in the geomaterial images. Fig. 2 (left) shows a representation of a 4 by 4 pixel image of an object containing two materials, identified each by integers 255 and 0; a DEM particle system, Fig. 2 (right) has been created with randomly-distributed particles in a square region of virtual space. The image data can be superimposed over the DEM system region by setting the points, in Cartesian coordinates, defining both regions to be coincident, i.e. $(P_{x1}, P_{y1}) = (P_{x3}, P_{y3})$ and $(P_{x2}, P_{y2}) = (P_{x4}, P_{y4})$. The dimensions of the grid spaces, Δ_x and Δ_y, are found by,

$$\Delta_x = \frac{P_{x2} - P_{x1}}{N_x}$$
$$\Delta_y = \frac{P_{y2} - P_{y1}}{N_y}, \qquad (1)$$

where N_x and N_y are the number of pixels in the x and y-directions, respectively. A particle whose centroid falls within a text image grid containing a certain integer value is flagged with that same integer value; subsequently, these integer flags determine which material property values to use in DEM systems with multiple types of minerals, e.g., particles flagged with the integer 255 are assigned mechanical properties consistent with a stiff material while flagging a particle with the integer 0 will assign the particle the properties of a more flexible material in this case. The choice of sizes of particles is described in Section 3.1, below.