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Representative elementary volume analysis of porous media using X-ray computed tomography

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ABSTRACT

The concept of representative elementary volume (REV) is critical to understand and predict the behaviour of effective parameters of complex heterogeneous media (e.g., soils) in a multiscale manner. Porosity is commonly used to define the REV of a given sample. In this paper we investigated whether the use of a REV for porosity can be used as a REV for other parameters such as particle size distribution, local void ratio and coordination number. X-ray computed tomography was used to obtain 3D images (i.e., volumes) of natural sand systems with different particle size distributions. 3D volumes of four different systems were obtained and a REV analysis was performed for these parameters utilizing robust 3D algorithms.
Findings revealed that the REV_{min} for porosity may not be adequate to be considered as a REV for parameters such as particle size distribution, local void ratio and coordination number. The REV_{min} for these parameters was observed to be larger than the REV_{min} for porosity. Heterogeneity of the systems was found to be an important factor to determine the REV for the parameters analyzed in this paper. The REV analysis revealed that as the uniformity coefficient increased, a larger volume was required to obtain the REV_{min} for the distribution of particle sizes and coordination number whereas a smaller volume was required to obtain the REV_{min} for local void ratio. Therefore, determination of the REV for parameters described in this paper or any microscale parameter of concern should not be derived based on REV for porosity and should be determined based on their distributions over different volumes.

1. Introduction

The scale of observation is an important aspect in modelling the behaviour of material (e.g., soil) or deriving its effective macroscale parameters from the constitutive relations that are governed by the spatial distribution of its components. A given soil sample can be considered homogenous when the scale of observation is large enough where parameters of concern are constant. Upon further increase of the spatial scale, soil parameters may become nonstationary [1,2].

Macro and multiscale modelling are two approaches commonly used to study the behaviour of materials and to predict effective macroscale parameters. In the macroscale modelling approach, the domain of concern is considered homogenous where assumptions regarding the microscale behaviour of materials are usually imposed to reach closed-form expressions [3–5]. In the multiscale approach, a coupled micro and macroscale analysis is performed where a microscale analysis is performed over volumes of finite sizes and results are then incorporated into macroscale formulations to evaluate effective macroscale parameters [6–8]. A key issue in both modelling approaches is the determination of a representative elementary volume (REV). The REV can be defined as the minimum volume of a soil sample from which a given parameter becomes independent of the size of the sample [9]. The size of an REV ranges from a minimum bound, which is the transition from the microscale to the macroscale level, to a maximum bound, which is the transition from a homogenous to a heterogeneous state.

There are two main approaches commonly used to determine the REV of a given sample for prediction and analysis of effective macroscale parameters. The first approach determines a REV based on porosity regardless of the macroscale parameter of concern (i.e., a sample is considered a REV if its porosity is constant over different sizes of the sample). This approach is common in soil science and hydrology literature. Clausnitzer and Hopmans [10] used porosity as a base to determine REV of ideal systems (i.e., glass beads packs). Other studies determined REVs of natural soil systems based on porosity [11–14]. A similar approach was used to determine representative elementary area (REA) for natural soil systems [15]. The second approach determines a REV based on macroscale parameters without prior determination of microscale parameters of the sample (e.g., porosity). This approach is commonly used in engineering mechanics literature. The sample is considered a REV when the macroscale under

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consideration is constant over different volumes. Macroscale parameters such as elastic modules and peak stress are common in determining the size of REV [16–20]. The determination of the REV size is by no means a trivial task as it is a function of the nature of the material being considered, the objective of the macroscale model and microscale parameters that impact the effective macroscale parameters. Moreover, the difficulty of microscale characterization of real porous media systems makes the determination of REV based on microscale parameters even more challenging.

It has been recognized that geometry and topology of soil particles control its thermal, fluid-like flow, stress transfer mechanisms and other mechanical parameters. For instance, mechanical conditions of a granular sand system such as shearing, compaction, transmission of stress and statistical parameters of contact force distribution are greatly influenced by its microscale characteristics (e.g., the distribution of the number of contacts of particles) [21–23]. Considering two adjacent particles within the assembly, one needs to account for the exact interaction characteristics so that the interparticle forces and relative motions can be estimated. The interparticle interaction is essentially controlled by sizes of particles and the nature of their contacts. Furthermore, the macroscale behaviour of granular assemblies such as fluid-like flow, stress–strain response and multi-phase flows (e.g., relative permeability) can be described by microscale models. Such models require determination of microscale parameters such as distributions of local void ratio, number of contacts and particle size.

The overall objective of this paper is to test whether parameters such as particle size distribution, local void ratio and coordination number are constant over a REV for porosity (i.e., can a REV for porosity be considered as REV for these microscale parameters?). This objective was achieved through the following steps: (1) use of X-ray microtomography to obtain non-destructive 3D images of different sand systems; (2) development of robust and efficient algorithms to compute pertinent parameters from 3D images at the microscale level; and (3) REV analysis of each microscale parameter to observe its correlation to the REV for porosity.

2. Materials and methods

2.1. Sand samples

Natural sand systems were prepared and used for imaging and REV analysis. To incorporate heterogeneity in the analysis, four different samples of the following particle sizes were used: 1.4 – 1.7 mm, 1.0 – 1.2 mm, 0.4 – 0.6 mm, and 0.4 – 1.7 mm. These samples were labeled in this paper as *S1*, *S2*, *S3* and *S4*, respectively. The sand was carefully packed under dry conditions in Perspex tubes (24 mm internal diameter and 10 cm height). Sand particles were poured into the tube through a funnel while continuously tapping the tube wall to ensure homogenous distribution of particles. To ensure repeatability of the packings, each system was packed and imaged three different times. Porosity values obtained from images of replicas of each system were identical. Porosity values obtained from images matched values obtained from laboratory measurements of porosity. Therefore, only one representative sample of each system was presented and analyzed in this paper.

2.2. X-ray computed tomography

Sand tubes were scanned using a Benchtop 160Xi (X-tek Ltd) cone-beam X-ray computed tomographer at 130 kV and 240 µA. A copper filter (0.5 mm thickness) was used to obstruct X-rays below 50 kV which typically contribute to noise in the acquired images. Each 2D projection collected by the X-ray intensifier (detector) consisted of an averaging of 64 radiographs obtained at every 0.294° projection angle, producing a total of 1225 projections for a 360° rotation and used to reconstruct the 3D volume. The maximum height and width of each scan is 49 mm and 28 mm, respectively. The size of each voxel of the reconstructed volume (i.e., the resolution) is (40 × 40 × 40 µm).

2.3. Image reconstruction and pre-processing

An image (3D volume) in this paper refers to a stack of reconstructed cross-sections (i.e., 2D slices) of the sample. Each cross-section was reconstructed by the filtered back-projection algorithm using the radiograph projections. In the reconstructed images, each voxel represents the mean linear attenuation coefficient of the corresponding resolved volume of the sample. Ring artifacts commonly appear close to the rotation axis due to noise in each projection. These were eliminated using a linear translation mechanism embedded in the 5-axis manipulator table of the X-ray CT equipment. Ring artifacts caused by pixels nonuniformity in the imaging device were eliminated using an image processing algorithm provided by CT scanner manufacturer. Beam hardening artifacts were insignificant in the images due to the use of a copper filter and the relative small size of the sample. Each projection was the average of a number of frames dependent on the X-ray flux (the higher the X-ray flux the less the number of frames required, 32 frames typically acquired for each radiograph in this study) which reduced errors caused by noise therefore increasing the quality of the reconstructed 3D volume.

Segmentation was used to convert 3D images to binary images by identifying two populations (i.e., phases) in the image based on their intensity values. In this paper we used the algorithm and software (i.e., 3DMA) described in Refs. [24–26] for image segmentation, the reader should refer to these references for more detailed description of the technique. Segmentation was performed using local thresholding values based on an indicator Kriging approach utilizing two threshold limits. Intensity values below the lower threshold were identified as one phase whereas intensity values larger than the higher threshold were identified as another phase. Values between the two thresholds were assigned to either phase using the maximum likelihood estimate of each phase based on the two-point correlation function. The accuracy of the segmentation algorithm was verified by comparing porosity values obtained from the images of the systems to the values obtained from laboratory measurements. This segmentation approach has also proven to be a very accurate and effective method of segmentation for different types of porous media systems (e.g., [13]).

Factors such as the existence of spots of extreme intensity values in the solid phase, segmentation process, and resolution of the image can generate small clusters of isolated voxels and small gaps in the solid phase in the binary image. Although such artifacts can be minimized by performing intensity scaling to the raw image and utilizing optimized thresholding values during the segmentation process, a few can still exist. In this paper, specific filters were implemented to remove small clusters of isolated voxels and fill artificial small gaps in the solid phase before any computations of microscale parameters. Top and bottom slices in the raw images of each sand system were removed since they contain noise due to the scanning process, extra rows and columns at boundaries of the raw images were also removed to improve the computational efficiency.

2.4. Microscale parameters

A brief description of the algorithms used to compute microscale parameters from 3D images is provided in the following sub-sections. A more detailed description can be found in Al-Raoush [27].

2.4.1. Recognition of individual particles

Identification of individual particles in a given sand image is the first step required to determine its microscale parameters. Particle