Particuology 27 (2016) 88–94

Contents lists available at ScienceDirect

Particuology

journal homepage: www.elsevier.com/locate/partic

Representative elementary volume analysis of polydisperse granular packings using discrete element method

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ARTICLE INFO

Article history:
Received 13 April 2015
Accepted 18 August 2015
Available online 25 October 2015

Keywords:
Representative elementary volume
Polydisperse packing
Discrete element method
Sample size effect

ABSTRACT

The representative elementary volume (REV) for three-dimensional polydisperse granular packings was determined using discrete element method simulations. Granular mixtures of various sizes and particle size distributions were poured into a cuboid chamber and subjected to uniaxial compression. Findings showed that the minimum REV for porosity was larger compared with the REV for parameters such as coordination number, effective elastic modulus, and pressure ratio. The minimum REV for porosity and other parameters was found to equal 15, 10, and 5 times the average grain diameter, respectively. A study of the influence of sample size on energy dissipation in random packing of spheres has also confirmed that the REV size is about 15 times the average grain diameter. The heterogeneity of systems was found to have no effect on the REV for the parameters of interest for the narrow range of coefficient of uniformity analyzed in this paper. As the REV approach is commonly applied in both experimental and numerical studies, determining minimum REV size for polydisperse granular packings remains a crucial issue.

Introduction

The representative elementary volume (REV) is the smallest volume over which the macroscopic mechanical behavior of a material can be defined in terms of averages. The REV concept, introduced by Bear (1972) and commonly applied in solid and granular mechanics, provides an effective means of developing macroscopic measures in the description of materials. It is critical in understanding and predicting the behavior of effective properties of complex heterogeneous materials at different scales (Razavi, Muhunthan, & Al Hattamleh, 2007; Adjémian & Evesque, 2001). Determining the REV size of heterogeneous materials is an important issue in macroscale and multiscale modeling (El Houdaigui, Forest, Gourgues, & Jeulin, 2006; Nguyen, Combe, Caillerie, & Desrues, 2014; Serafin & Cecot, 2013), which are two approaches commonly used to estimate properties of heterogeneous materials.

There are two most-frequently applied methods for determining the REV size of samples for predictions of effective macroscale parameters. A method, common in soil science and hydrology literature (Brown, Hsieh, & Lucero, 2000), is a minimum REV of a sample over which porosity remains constant. Fig. 1 shows a conceptual schematic representing the idealized relationship between porosity and the volume of a porous media, proposed by Bear (1972). For a very small elementary volume (region I), porosity fluctuates strongly, which is associated with pore scale heterogeneity. As elementary volume increases, fluctuations in porosity decrease, until above some value V_{min} when only small amplitude fluctuations around constant value of porosity occur (region II). For homogeneous porous media, a minimum REV is defined as the left-hand boundary of region II. The porosity measurements made in this region are scale-independent and accurately represent a larger system. A further increase in volume of the porous medium above value V_{max} may result in an increase in heterogeneity, related to 'macroscopic' volume features (region III). For heterogeneous porous media, the REV theoretically lies between regions I and III; however the determination of region II for real heterogeneous systems may be difficult (Zhang, Zhang, Chen, & Soll, 2000).

The second method for determining the REV size of a sample, commonly applied in engineering mechanics, is based only on macroscale parameters discounting microscale parameters of the sample, such as porosity. The sample is considered a minimum REV when the macroscale parameter, e.g., elastic modules and peak stress (Shan & Gokhale, 2002; Graham & Yang, 2003), remains constant over different sizes.

In recent years, a number of papers have dealt with the estimation of REVs of porous materials using experimental (Zhang et al., 2000; Razavi et al., 2007; Al-Raoush & Papadopoulos,

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http://dx.doi.org/10.1016/j.partic.2015.08.004

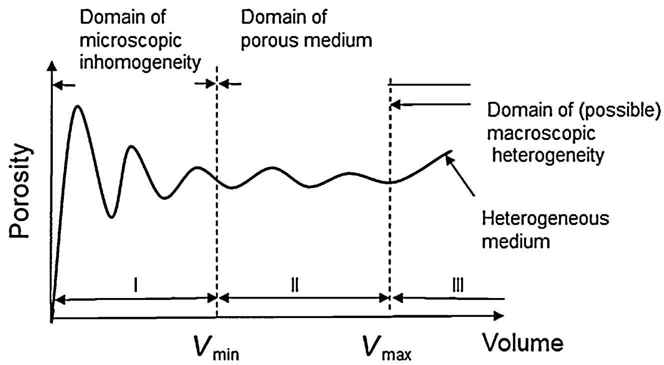

Fig. 1. Conceptual schematic representing the idealized relationship between porosity (φ) and volume (V) of porous media. Modified after Bachmat and Bear (1987).

2010; Costanza-Robinson, Estabrook, & Fouhey, 2011), theoretical (Bachmat & Bear, 1987), and numerical methods (Evesque, 1991; El Houdaigui et al., 2006; El Houdaigui, Forest, Gourgues, & Jeulin, 2007; Ukrainczyk & Koenders, 2014). The most commonly applied techniques are X-ray microtomography (Razavi et al., 2007; Al-Raoush & Papadopoulos, 2010; Costanza-Robinson et al., 2011) and computational techniques based on the finite element method (FEM) (Evesque, 1991; El Houdaigui et al., 2006; Tejchman & Górski, 2008; Nguyen et al., 2014) and discrete element method (DEM) (Adjémian & Evesque, 2001; Norouzi, Baghbanan, & Khani, 2013; Nguyen et al., 2014). These studies have shown that the minimum REV size varies depending on the considered material and the physical quantity of interest (Evesque, 2001; Gitman, Gitman, & Askes, 2006; Razavi et al., 2007; Costanza-Robinson et al., 2011; Norouzi et al., 2013; Nguyen et al., 2014; Ukrainczyk & Koenders, 2014). Razavi et al. (2007) reported that fewer grain diameters were required to achieve REV for glass beads than for natural media with similar grain-size distributions. This difference was probably due to the smooth glass beads slipping past each other more readily than rough irregularly-shaped natural grains, which allowed beads to achieve a more uniform arrangement during the column packing.

The REV is related to either the mean grain diameter or the diameter of the largest particle of the porous medium. Based on extensive experience, the authors of Eurocode 1 (EN 1991–4:2006) recommended the diameter for the direct shear cell to be 20 times the largest particle size. Masson and Martinez (2000) showed that a sample size equal to 7 to 8 times the size of the largest particle was sufficient to obtain a REV size for porosity and coordination number whereas 12 times the largest particle size was required for proper stress tensor evaluation. These results were in agreement with experimental data of Lanier and Jean (2000), Biarez and Hicher (1994), and Rusinek, Molenda, Sykut, Pits, and Tys (2007).

Evesque (2001) reported that the minimum REV size in most granular experiments and computer simulations corresponded to two or three grain diameters, but may be higher in some cases. The avalanche experiments conducted by Evesque (1991) and Held et al. (1990) provided evidence for a much larger REV size, equal to about forty grain diameters. The study by Adjémian and Evesque (2001) of the stick-slip mechanism in glass spheres subjected to uniaxial compression has shown that the minimum representative sample was 10^7 grains.

A finite element study by Gitman et al. (2006) of the REV size dependence on various parameters relevant to random heterogeneous granular materials subjected to tension and shear tests has shown only a slight effect of the loading scheme and the parameter of interest (stress-based or stiffness-based). However, a strong dependence of the REV size on the changing material properties such as Young's modulus was observed.

The application of X-ray computed tomography by Al-Raoush and Papadopoulos (2010) and Costanza-Robinson et al. (2011) to obtain images of sand systems with different particle size distributions provided information about dependence of REV size on grain-size distribution. These authors observed that as the particle size distribution increased, a larger REV size was required for porosity and coordination number. They also found that the REV for porosity is smaller than those for particle size distribution, local void ratio, and coordination number. Therefore, the REV size for porosity should not be considered as a REV for these parameters.

The large-scale application and processing of granular materials in many branches of industry requires improved insight into the complex nature of particulate assemblies; however, due to difficulties associated with the measurement and characterization of granular microstructure, the determination of REV size for granular packings remains an open issue.

The majority of particle packings involved in industrial and natural processes involve particles of a broad range of particle sizes. The degree of particle-size heterogeneity determines the geometric and micromechanical properties of packings. These properties strongly affect its mechanical response to external loads during shearing (Voivret, Radjai, Delenne, & El Youssoufi, 2009), compaction (Zhang & Napier-Munn, 1995; Bentham, Dutt, Hancock, & Elliott, 2005; Wiącek & Molenda, 2014b), and discharge processes (Gundogdu, 2004). Many studies on REV size for polydisperse porous materials refer to geometric parameters (e.g., porosity, local void ratio, and coordination number) or permeability parameters (e.g., moisture saturation), which are of interest to geotechnical engineers; however, the issue of the minimum REV for mechanical parameters remains unsolved.

Therefore, in our study, we performed numerical simulations with the goal of estimating the minimum REV size for polydisperse granular packings with various particle size distributions and understanding the dependence of the REV size on the parameters of interest (porosity, coordination number, elastic modulus, and pressure ratio).

Numerical method

Discrete element method

The DEM, based on a microstructural approach (Cundall & Strack, 1979), with the non-linear Hertz–Mindlin contact model was applied to model granular packings. The viscoelastic contact between particles may be presented by a system composed of an elastic spring and viscous damper in the normal direction, and spring, damper, and frictional slider in the tangential direction (Wiącek & Molenda, 2014a). The spring models the accumulation of elastic energy in the system, whereas the damper and slider model the dissipation of energy. We model the particle interactions assuming a soft contact between rigid particles by allowing overlaps at the point of contact.

The detection of such contacts is followed by a calculation of the normal (F^n) and tangential (F^t) contact forces at each incremental time step, given by

$$F^n = k_n \delta_n^{3/2}, \quad (1)$$

$$F^t = -k_t \delta_t, \quad (2)$$

where k_n and k_t are the normal and tangential stiffness coefficients, and δ_n and δ_t are the normal and tangential cumulative shear displacements. The stiffness coefficients may be expressed as

$$k_n = \frac{4}{3} Y^* \sqrt{R^*}, \quad (3)$$

$$k_t = 8G^* \sqrt{R^* \delta_n}, \quad (4)$$