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Effect of particle size distribution on micro- and macromechanical response of granular packings under compression

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ABSTRACT

The role of particle size heterogeneity on micro- and macromechanical properties of assemblies of spherical particles was studied using DEM simulations. The response to an imposed load of a granular material composed of non-uniformly sized spheres subjected to uniaxial confined compression was investigated. A range of geometrical and micro-mechanical properties of granular packings (e.g., void fraction, contact force distribution, average coordination number and degree of mobilisation of friction at contacts between particles) were examined, and provided a more accurate interpretation of the macroscopic behaviour of mixtures than has previously been available. The macromechanical study included stress transmission, stiffness and angle of internal friction of the granular assemblies.

The degree of polydispersity showed slight effect on both, the void fraction and the elastic properties of the system. The tendency for increase in the lateral-to-vertical pressure ratios was observed with an increasing degree of particle size heterogeneity; however, the different pressure ratios calculated for samples with various degrees of polydispersity lay within the range of data scatter.

1. Introduction

Transporting, storage and processing materials in granular form are common operations in many industries, including the agriculture and food industries, and the pharmaceutical, cosmetics and building industries. Granular materials play an important role in chemical engineering and processes that deal with chemical powders and granules. Materials are subjected to technological processes such as compression and mixing, whose designs require advanced research into the properties of granular matter. In mechanics and physics, two ways may be distinguished for describing and modelling particulate, heterogeneous materials such as powders or grains (Luding et al., 2005). The first approach, based on continuum theory, describes the macroscopic behaviour of a material, which is completed by a microscopic description of the material in which the particles and their interactions are modeled at a particle scale. The macroscopic approach involves stress, strain and plastic yield conditions. The microscopic approach addresses the local force–deformation laws for each particle contact. Relating the micro-mechanical properties of a particulate system to its macroscopic behaviour requires a description of the fabric of the material. In turn, quantification of the fabric requires information regarding the number of contacts and the spatial distribution of contact orientations in the packing in order to relate contact forces to stress, and displacements to strains. The macromechanical response of a particulate assembly to external shear forces (Voivret et al., 2009), compaction forces (Ma and Zhang, 2006; Zhang and Napier-Munn, 1995; Zhou et al., 2005), mixing forces (Remy et al., 2011) or discharge processes (Gundogdu, 2004) has been reported to be closely related to the micromechanical properties of the granular system, which are determined by the interactions between the particles in the system. The mutual rearrangement of particles affects the coordination number (*CN*), the contact area and the transmission of stress in granular packings. Martin et al. (2003) observed that, for isostatic compaction and closed-die compaction modelled by the discrete element method (DEM), the average *CN* increased and the average contact area decreased, while concurrently the distribution of contact area values broadened. DEM simulations of uniaxial compression of pebble beds conducted by Gan and Kamlah (2010) provided information on micro–macro relationships in particulate assemblies. The microscopic information, such as the maximum contact force and the *CN* inside the assembly, were related to the macroscopic stress variables. Gan and Kamlah (2010) reported a large increase in the average *CN* as compressive stresses increased in the low stress region, due to the rearrangement of particles during

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loading; new contacts were formed in the compressed state, which in turn increased the stiffness of the assembly.

Studies of the mechanical properties of granular packings have mainly been related to monodisperse systems; however, most particulate materials in industrial and natural processes comprise particles in a broad range of sizes. The polydispersity of a system of particles affects the rearrangement of the particles and their contact network in granular systems, such that particulate materials and powders have different compaction characteristics. This is very important in the chemical and pharmaceutical tablet manufacturing industries (Reaple et al., 2007). Voivret et al. (2007) reported that the degree of particle size heterogeneity affected the geometrical aspects of packing characteristics and micro-mechanical properties, which then determined the way in which contact forces were transmitted in granular systems. They observed that increased particle size polydispersity transformed the disorder from a state where particle connectivity governed packing properties to one where pore-filling small particles prevailed, and also a less anisotropic fabric with an extended particle size distribution.

Bentham et al. (2005) used numerical simulations to study the geometrical and mechanical characteristics of uniaxially compressed polydisperse packings of spheres. They found that the contact number and the distributions of normal contact forces were both broader for mixtures with more highly dispersed particle diameters. Wiącek and Molenda (2013) observed increases in both the homogeneity of distribution of normal contact forces and the anisotropy of the contact network, together with increasing standard deviation of particle mean diameter, in polydisperse mixtures of spheres. They found a relationship between the degree of polydispersity of granular packing and the dissipation of energy in such systems. Laboratory tests and numerical simulations were conducted by O'Sullivan et al. (2002) on biaxially compressed circular-section steel rods whose radii had a relatively low standard deviation. They observed a change in the strength of samples with increasing particle-size polydispersity and decreasing average coordination number.

Kruyt and Rothenburg (2001) carried out a micro-mechanical DEM investigation of polydisperse assemblies of discs subjected to compression and shearing. This showed that the probability functions for the normal component of the vectors connecting the centres of particles in contact resembled a lognormal particle size distribution, and the coordination number of the particles was linearly related to their radius.

A review of the literature shows that the macroscopic behaviour of a particulate assembly is strongly related to its microscopic properties, which themselves are determined, *inter alia*, by the degree of polydispersity of the granular packing. Microstructural characterisation of particulate media is critical for understanding and predicting the macromechanical response of particulate assemblies to loads applied during mechanical processes. These responses, in turn, determine the efficiency of the process as well as the quality and safety of the product. Most particle packings in industrial and natural processes are composed of particles that are non-uniform in size; therefore the study of micro–macro relations in polydisperse granular systems is of great interest to researchers in the field. It seems from the literature that insufficient studies have been done on the relationship between the extent of particle size variation and the geometrical and mechanical properties of granular materials, especially for highly polydisperse particulate packings. The objective of the present study, therefore, was to investigate the responses to uniaxial compression of assemblies of spheres with wide ranges of standard deviation of their mean diameter, and the effect of such particle size heterogeneity on the micro- and macromechanical properties of the assembly. The data used in this study were obtained by performing three-dimensional DEM simulations.

The outline of this paper is as follows. In Section 2, the DEM and model used here are described. The predicted micromechanical and macromechanical properties of polydisperse assemblies of spherical particles, and discussion, are presented in Section 3. Conclusions drawn from the work are presented in Section 4.

2. Model description

The discrete element method (DEM), based on a microstructural approach (Cundall and Strack, 1979), is a numerical technique commonly used for detailed investigation of the mechanical behaviour of granular systems. The simplified non-linear Hertz-Mindlin contact model of Ji and Shen (2004) was used. This model supposes an elastic spring and a viscous damper in the normal direction, and a spring, damper and frictional slider in the tangential direction. The spring is analogous to the accumulation of elastic energy in the system as the applied load increases; the damper and slider simulate energy dissipation. The detection of contacts between the particles is followed by calculation of the normal and tangential forces at these contacts, at each incremental time step; the time increments are small enough to allow an assumption of constant translational and rotational accelerations. The motion of each particle in the system is given by Newton's equations of motion. These are integrated to provide information about individual particles' positions and velocities, and the resultant forces exerted on each particle. The contact-point behaviour adopts a "soft contact" approach, which permits local overlap of rigid particles at contact points. The tangential contact force is limited by the Coulomb friction law, which assumes that particles slide over each other when the magnitude of the tangential force equals or exceeds some limiting value.

In this study, three-dimensional DEM simulations were conducted using the EDEM program (EDEM Software). Polydisperse mixtures of spheres were poured into a test chamber of rectangular cross-section $0.12\ \mathrm{m} \times 0.12\ \mathrm{m} \times 0.132\ \mathrm{m}$ (Fig. 1). The walls of chamber were a rigid frictional boundaries that did not deform under the applied load. The assumption of rigidity of the walls was required to derive equations for mechanical parameters of material analysed in this study. The dimensions of the sample were greater than 15 mean particle diameters (D_m). The slight changes in the void fraction (Φ) and effective elastic modulus (E) with increase in thickness of sample from $15D_m$ to $20D_m$ (Fig. 2) allow the dimensions of the sample greater than 15 mean particle diameters to be regarded as a representative elementary volume. The decrease in the dimensions of the simulation cell or increase in dimensions of spheres would result in large disturbances of stress field from the walls of the apparatus, while a decrease in dimensions of spheres below certain value would result in change in physical interactions in contacts.

The diameter of the basic sphere was 7.3 mm. The normal particle size distribution with various standard deviations (*s.d.*) was varied in the model such that the *s.d.* of the particle mean diameter ranged from 0% to 80%. Increasing the *s.d.* of the mean particle diameter resulted in a predicted decrease in the number of spheres in a chamber of fixed volume from 4800 in packings with *s.d.* = 0%, 20% and 40% to 4000 in those with *s.d.* = 60%, and down to 2350 in highly polydisperse mixtures. The input parameters for the DEM simulations are listed in Table 1 (e-Funda, 2014; Wiącek, 2008). In spite of the assumption of rigidity of the walls of test chamber, Table 1 shows also the elastic constants of wall material, required to calculate forces exerted on the wall by contacting particles.

In the first stage of the simulation, particles were randomly generated in a box measuring $0.12 \times 0.24 \times 0.132$ m. The granules then settled to the bottom of the rigid test chamber under the influence of gravity. The initial configurations of the monodisperse