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Effect of number of granulometric fractions on structure and micromechanics of compressed granular packings

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ABSTRACT

The role of number of grain size fractions on structural and mechanical properties of uniaxially compressed granular packings with a uniform particle size distribution in terms of number of particles and with various particle size dispersities was studied using the discrete element method. The study addressed packing density, coordination number, contact forces, global stress, and energy dissipation in assemblies composed of frictional spheres. Packing density was found to change with increasing number of granulometric fractions in mixtures with a small ratio of the diameters of the largest to smallest particles. Results indicated a certain value of particle size ratio below which the number of particle size fractions strongly affected packing density. The average coordination number decreased with increasing number of fractions. Detailed analysis of the effect of particle size dispersity on mechanical coordination number, including particles with no less than four contacts, revealed that, contrary to the average coordination number, the mechanical coordination number increased with increasing ratio of the diameters of the largest to smallest particles in the sample. The composition of polydisperse samples strongly affected stress distribution and energy dissipation in granular packings.

Introduction

Polydisperse granular materials exhibit complex and undefined behavior, posing considerable challenges in the design and operation of processing plants. Granular packings may be composed of one, two, three, or more components that differ from one another in size, shape, and material properties. Size polydispersity is an inevitable feature of granular materials that determines structural and mechanical properties of particulate systems. Size characterization of particles and its influence on the mechanical response of grain assemblies subjected to various processes is of key interest in various fields of science and engineering. This issue is of particular importance for the chemical and pharmaceutical industries, in which numerous processes involve granular materials composed of non-uniformly sized particles.

Numerous studies have been performed on the properties of polydisperse granular packings during the last few decades. These reveal a high dependence of structural and mechanical properties of particulate systems on geometric factors (e.g., particle size ratio, degree of particle size heterogeneity) and their statistical distributions (e.g., volume fraction of particle size fractions, shape of particle size distribution) (Abou-Chakra & Tüzün, 1999; Dorai et al., 2015; Dutt & Elliott, 2014; Göncü, Durán, & Luding, 2010; Hwang, Wu, & Lu, 1997; Jalali & Li, 2007; Martin & Bouvard, 2004; McGeary, 1961; O'Sullivan, Bray, & Riemer, 2002; Ramachandran et al., 2012; Rassouly, 1999; Shaebani, Madadi, Luding, & Wolf, 2012; Skrinjar & Larsson, 2004; Thornton, 2010; Voivret, Radjai, Delenne, & El Youssoufi, 2007; Wiącek & Molenda, 2014a, 2014b). An experimental study conducted by McGeary (1961) using binary granular packings of spheres showed a strong relationship between packing density of the particulate assembly and both the particle size ratio and volume fractions of particles representing various grain size fractions. This author observed an increase in packing density as the volume fraction of small particles increased to 60%; further increase in the contribution of small particles to the mixture resulted in a decrease in packing density of the sample. These findings were later confirmed by the theoretical calculations of Rassouly (1999) and numerical results obtained by Martin and Bouvard (2004), Jalali and Li (2007), and Wiącek (2016).

A study of the structural properties of bimodal mixtures, conducted by Skrinjar and Larsson (2004), revealed a decrease in the average coordination number with increasing number of small particles in compressed sphere packings. Wiącek (2016) observed that the relationships between average coordination number and volume fraction of small particles followed the trends similar to those of solid fraction–volume fraction of small particles curves,

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indicating a strong relationship between the coordination number and the solid fraction of binary mixtures. In packings comprising similarly sized particles, with a ratio of the diameters of large to small spheres of 1.2, a slight effect of small components on the number of contacts between particles was observed. In packings with larger particle size ratios, the average coordination number increased with increasing number of small grains and reached a maximum when the volume fraction of small particles was 60%; further increase in the number of small particles in an assembly resulted in a decrease in the average number of contacts between grains. An increase in the average coordination number with an increase in volume percentage of small particles in bimodal mixtures was also observed by Martin and Bouvard (2004). A study of the mechanical response of isostatically compacted binary packings, conducted by these authors, revealed a stiffer response of mixtures with a smaller volume fraction of small particles and larger particle size ratio.

Numerical studies on structural properties of highly polydisperse packings with various size distributions, carried out by Hwang et al. (1997) and Roozbahani, Huat, and Asadi (2013), revealed a strong relationship between packing density and the shape of the particle size distribution (PSD). A detailed analysis of microstructure and micromechanical characteristics of three-dimensional granular materials with continuous normal, log–normal, and arbitrary PSDs, conducted by Wiącek and Molenda (2014c), showed slight differences between properties of the specimens; however, comparing results obtained for samples with discrete uniform and continuous PSDs, it was evident that the former provided smaller packing density, resulting in different micromechanical characteristics of the mixtures.

Extensive studies of granular packings with various degrees of particle size heterogeneity, performed inter alia by O'Sullivan et al. (2002), Voivret et al. (2007), Göncü et al. (2010), Shaebani et al. (2012), Wiącek and Molenda (2014b), and Dutt and Elliott (2014), have shown that the degree of polydispersity of a mixture also determines its structure and mechanical characteristics. O'Sullivan et al. (2002) observed that the strength of hexagonally packed rods subjected to biaxial compression decreased significantly with an increase in the standard deviation of the rod sizes. A numerical study by Voivret et al. (2007) on the space-filling properties of polydisperse two-dimensional granular packings showed that the solid fraction increased with increasing degree of polydispersity of the grain assembly. These authors indicated a strong relationship between the degree of particle size heterogeneity and anisotropy of the contact network in the sample. A theoretical study conducted by Shaebani et al. (2012) for polydisperse granular materials showed that the trace of fabric and stress tensors was determined by the mean packing properties (packing fraction, average coordination number, and average normal contact force) and correction factors that depended on the moments of the PSDs; nevertheless, these authors considered the elastic moduli of polydisperse packings to be independent of degree of particle size heterogeneity. A strong relationship between the degree of particle size polydispersity and the micromechanical properties of three-dimensional spherical packings was found by Göncü et al. (2010) and Wiącek and Molenda (2014b), who observed a decrease in pressure in granular packings with increasing standard deviation of the mean particle diameter. Wiącek and Molenda (2014b) found that the average coordination number and anisotropy of the contact normal orientation decreased as particle size heterogeneity increased.

Karion and Hunt (1999) observed an increased rate of energy dissipation during gravity-free Couette flow of binary granular packings when the ratio of the diameters of large to small granules increased. The greater energy dissipation in systems composed of larger granules was related to the ratio of the proportion of energy dissipated in collisions to the mass of the colliding bodies. A strong relationship between degree of particle size dispersity and value of energy dissipated in granular mixtures with a normal PSD was reported by Wiącek and Molenda (2014b), who observed higher dissipation of energy in more heterogeneous mixtures. Granular dynamic simulations of uniaxial compression, conducted by Dutt and Elliott (2014) for spherical packings with a discrete non-uniform PSD and various numbers of grain size fractions, showed a decrease in packing fraction and average coordination number with an increase in the ratio of the diameters of the largest to smallest particles in the system. No significant variation in the stress response of granular assemblies at small strains was observed; however, at larger strains, mixtures with higher grain size dispersity were softer.

Structural and micromechanical properties of particulate systems were proven to determine macro-scale mechanical response of materials (Antony & Ghadiri, 2001; Bentham, Dutt, Hancock, & Elliott, 2005; Kumar, Imole, Magnanimo, & Luding, 2014; O'Sullivan et al., 2002; Voivret, Radjai, Delenne, & El Youssoufi, 2009; Wiącek & Molenda, 2014a; Zhang & Napier-Munn, 1995; Zhou, Advani, & Wetzel, 2005); therefore, in-depth insight into the nature of simple particulate systems is required to enable more accurate interpretation and prediction of effects observed in more complex packings. The above review of literature shows that extensive studies have been aimed at the characterization of polydisperse granular materials with different PSDs, many of which considered packings with a uniform discrete PSD. Although much research has been devoted to examination of binary or ternary grain assemblies with different size ratios, knowledge of the effect of number of grain size fractions on structural and micromechanical properties of materials with discrete PSDs is still very scarce. A large number of industrial processes involve granular materials comprising particles of different size fractions, so advancement of knowledge in this field is required to improve and optimize technological processes. No study of the effect of number of granulometric fractions on structure and mechanical characteristics of grain assemblies with uniform PSD has yet been undertaken; thus, the objective of the present project was to analyze the effect of number of particle size fractions on the structural and mechanical properties of granular mixtures composed of spheres with a size distribution uniform by number of grains. The study was conducted for mixtures with various ratios of diameters of the largest to smallest particles to verify whether the value of the particle size ratio has an influence on the relationship between the number of fractions and the structure and micromechanics of granular packings. Simple granular packings composed of three, five, and seven granulometric fractions were examined. After binary systems, these are the simplest polydisperse particulate systems. The study was restricted to specimens comprising a small number of particle size fractions to decrease the degree of complexity of the systems and to facilitate interpretation of the obtained results.

Materials and methods

Numerical simulations

Three-dimensional simulations were conducted using EDEM software (EDEM Software, 2016), which is based on the discrete element method (DEM) (Cundall & Strack, 1979). A simplified viscous–elastic non-linear Hertz–Mindlin contact model was used, wherein the normal contact force (F_{ij}^{n}), resulting from the contact of particle *i* with particle *j*, is expressed as:

$$F_{ij}^{\mathrm{n}} = k_{\mathrm{n}}\delta_{\mathrm{n}}^{3/2} - 2\sqrt{\frac{5}{4}}\beta\sqrt{k_{\mathrm{n}}m*}V_{\mathrm{n}}^{\mathrm{rel}}\delta_{\mathrm{n}}^{1/4}. \quad (1)$$