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Microstructure and micromechanics of polydisperse granular materials: Effect of the shape of particle size distribution

Joanna Wiącek *,[1], Marek Molenda [1]

Institute of Agrophysics, Polish Academy of Sciences, Doswiadczalna 4, 20-290 Lublin 27, Poland

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ABSTRACT

The uniaxial compression of polydisperse spheres with continuous: normal, log-normal, arbitrary and discrete uniform particle size distribution was modelled with the discrete element method (DEM). The evolution of solid fraction, coordination number and fabric tensor with increasing compressive stress was investigated in granular packings of equal mean particle diameter and standard deviation of particle mean diameter. The study of the relationship between the shape of particle size distribution and the micromechanical properties of granular packings included the determination of the contact forces and the degree of mobilisation of friction in contacts between particles. Slight influence of the shape of continuous particle size distribution on the solid fraction and coordination number in polydisperse packings was observed. The discrete uniform distribution provided the number of contacts lower by 7% as compared to continuous distribution. Concerning the mobilisation of friction in contacts between spheres, the average ratio of the tangential: normal contact forces in packing with discrete distribution was 25% higher than the one calculated for normal particle size distribution.

1. Introduction

The polydispersity of particulate system is one of the physical attributes of granular materials which determine their fabric and micromechanics [1–3]. The term *fabric* denotes the physical constitution of a granular material as expressed by the spatial arrangement of the particles and associated voids [4] which is of great importance in many branches of science and technology. Many scientific papers dealing with the microstructure of packings of ideal uniformly sized spheres have been published over the past several decades [5–7], however the most particle packings involved in the industrial and natural processes are composed of a broad range of particle sizes. The degree of particle size heterogeneity was found to determine the geometrical and micromechanical properties of packings, which in turn strongly affected their mechanical response to shear [1] or compaction [8,9] as well as the segregation and flow of particle mixtures during mixing [10] and discharge processes [11]. In general, the research on polydisperse particulate systems focused on the study of relationship between degree of polydispersity of packings and their mechanical properties [1,3]. The particle size distribution may be described by various distribution functions which were reported to determine porosity and coordination number in granular packings [12–14]. In the majority of investigations carried out in that field the Gaussian (normal) or log-normal particle size distributions were applied [15–17]. These two distributions are most often assumed to describe the random variation that occurs in the data from many scientific disciplines [18–20], however other distributions, such as exponential, arbitrary, bimodal, uniform or Rossin–Rammler may be also applied to describe the particle size distribution in particulate systems [13,15]. Understanding the relationship between particle size distribution and micromechanical properties of granular packings is of high importance to many branches of industry in which granular materials are processed, e.g. pharmaceutical, chemical, building or ceramics industry. Microstructure characterization of particulate media is critical to understand and predict their macromechanical response to loads applied during mechanical processes that in turn affects efficiency of the process as well as quality and safety of products.

Due to insufficient knowledge on the microstructure and micromechanical properties of particulate assemblies, resulting from limitations of experimental methods, computational approaches are increasingly preferred to represent granular media. In mechanics and physics, the description and modelling of heterogeneous particulate materials such as powders or grains may be done in two ways [21]. The first one, based on continuum theory, relies on empirical assumptions about the macroscopic material behaviour and involves stress, strain and plastic yield conditions. In the second approach, the macroscopic analysis is complemented by a microscopic description of the material in which individual particles and their interactions are modelled. Although both approaches have gained widespread application in the physics and mechanics of granular materials [22–25] the micromechanical approaches, which take into account the

* Corresponding author.
E-mail addresses: jwiacek@ipan.lublin.pl (J. Wiącek), mmolenda@ipan.lublin.pl (M. Molenda).
[1] Tel.: +48 81 744 50 61.

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discrete nature of the particulate system, are commonly preferred to continuum-mechanical approaches.

Numerous two- and three-dimensional models, based on micromechanical approaches, have been proposed to simulate the polydisperse packings of particles [12,26,27,14].

Suzuki and Oshima [28] investigated the relation between the coordination numbers and the shape of particle size distributions in mixtures of randomly packed spheres with log-normal, log-uniform, Rosin–Rammler and Andreasen (Gaudin–Schuhmann) distributions. They found that an average coordination number is close to 6 which is the value for a uniform-sized sphere bed, and it is independent on the type of size distribution. Hwang et al. [12] simulated the two-dimensional packing structures for circular and ellipsoidal particles with normal, Rosin–Rammler and uniform size distributions. In these simulations, the mean particle size and standard deviation of particle mean diameter were set to be the same. The authors showed significant influence of the shape of particle size distribution on packing porosity and the average coordination number in system. For ellipsoidal particles uniform distribution provided the highest porosity and the lowest porosity was observed in system with normal distribution. The study by Roozbahani et al. [14] of the effect of shape of particle size distributions on the porosity in multi-sized sphere packings with the same size range and normal, exponential, log-normal and arbitrary size distributions indicated that log-normal distribution of diameters of spheres provided the lowest value of porosity among all the distributions. The highest porosity was observed in samples with arbitrary particle size distribution.

The three-dimensional molecular-dynamics simulations of unbounded shear flows were conducted by Dahl et al. [15] to investigate the stresses and granular energy in granular materials with Gaussian and lognormal size distributions. The shear stress and pressure in mixtures were found similar to the ones predicted by monodisperse kinetic theory and independent on the width of particle size distribution. This width-independent nature of the total stresses was traced to an effective balancing of the stresses between the larger particles, which generate relatively high stresses, and smaller particles, which generate lower stresses. Moreover, the granular energy in Gaussian and lognormal systems was found to be unequally distributed among the various sizes of particles, with large particles possessing more granular energy than their smaller counterparts.

Earlier performed investigations have shown that microstructural properties of granular assembly are strongly affected by the width of particle size distribution, however description of fabric and micromechanical behaviour of granular deposits with various particle size distributions is still far from being complete. Although many studies on the fabric of particulate systems have been published over the past several decades, more insight is necessary to understand the relationship between microstructure and micromechanical properties of granular packings. Thus, the objective of the reported project was to examine relationship between characteristics of microstructure of the polydisperse granular packing and its behaviour under mechanical load. This knowledge is valuable for design of process equipment as well as for control of technological operations.

2. Simulation method

2.1. Discrete element method

Discrete element method (DEM), based on a microstructural approach [29], with the non-linear Hertz–Mindlin contact model was applied to model uniaxial compression tests of granular packings. The viscoelastic contact between particles may be presented by the set composed by an elastic spring and viscous damper in the normal direction, and spring, damper and frictional slider in the tangential direction [3]. Spring models accumulation of elastic energy in the system, whilst damper and slider model the energy dissipation.

Detection of contacts between particles is followed by calculation of the normal (F^n) and tangential (F^t) contact forces at each incremental time step, given by:

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

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

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

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

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

where Y^* is the equivalent Young's modulus; R^* is the effective radius of contacting particles; and G^* is an equivalent shear modulus. The time step is set to be small to allow the assumption of constant translational and rotational accelerations. The motion of each particle in system is given by Newton's equations. The integration of the equations of motion provides information regarding the particle's position, velocity and resultant forces. The rigid particles are allowed to overlap locally at contact points using a soft contact approach. The friction on sliding particles obeys Coulomb's friction law, expressed as:

$$F^t < \mu_s |F^n|, \quad (7)$$

where μ_s is the coefficient of static friction. The Coulomb friction law assumes that particles slide over each other when the tangential force is at limiting friction.

2.2. Sample preparation and input parameters

Three-dimensional DEM simulations were conducted using the EDEM software [30]. Polydisperse spheres with continuous and discrete particle size distributions were poured into a test chamber of rectangular cross-section 0.12 m × 0.132 m × 0.12 m (see Fig. 1). The dimensions of the sample were greater than 15 mean diameters ($\overline{D}$), which was regarded to be a representative elementary volume for polydisperse mixtures. The diameter of the basic sphere (D_b) was 7.3 mm. The number of particles in chamber of fixed dimensions varied from 4200 in the samples with log-normal and uniform distributions, to 4800 in packings with normal and arbitrary distributions. The input parameters for the DEM simulations are listed in Table 1.

The particles with random initial coordinates generated in the box measuring 0.12 m × 0.132 m × 0.25 m settled down onto the bottom of the test chamber under the influence of gravity. As soon as an equilibrium state was reached after deposition in uncompressed specimens,

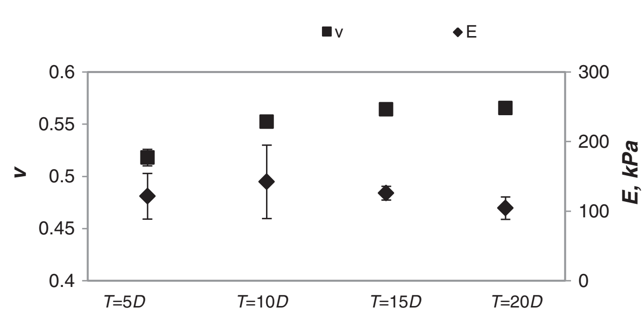

Fig. 1. Initial configuration of polydisperse sample with normal particle size distribution.