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DEM SIMULATIONS OF THE FRICTIONAL AND FRICTIONLESS POLYDISPERSE PACKINGS OF SPHERES UNDER UNIAXIAL COMPRESSION

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Abstract. The uniaxial compression of polydisperse assemblies of spherical frictional and frictionless particles is modeled with the discrete element method (DEM). The normal particle size distribution with standard deviation of particle mean diameter in the range from 0% to 80% was applied. The series of numerical tests have been conducted to study the micromechanical and macromechanical properties of packings of spheres. The micro-scale analyses included distribution of contact forces and average coordination number, whereas macromechanical study included the elasticity, stress transmission and angle of internal friction in the assemblies. The linear increase in solid fraction was observed for standard deviation of particle mean diameter increasing up to 50% in assemblies of both, frictional and frictionless spheres under pressure of 100kPa. Further increase in particle size heterogeneity decreased solid fraction in systems. The increase in coefficient of interparticle friction resulted in decrease in solid fraction by above 10% in the whole range of variability of *SD* value due to the different space-filling properties of frictional particles. The stiffness of samples increased with compressive loads increasing, however no clear effect of particle size polydispersity on the effective elastic modulus of mixtures was found in frictional sphere packings. The effective elastic modulus increased with *SD* value increasing up to 50% in sample composed of smooth particles that decreased for higher *SD* values. Discrete element method predicted decrease in pressure ratio with standard deviation of particle mean diameter increasing up to 50%. Further increase in particle size polydispersity increased value of the parameter. Increase in coefficient of interparticle friction to 0.4 resulted in about 40% decrease in pressure ratio in sphere packings.

1 INTRODUCTION

A granular material is a collection of distinct macroscopic particles which exhibits complex behavior, very different from ordinary solids and fluids and which is of high interest from researchers and industry. The majority of particle packings involved in industrial and natural processes are nonuniformly sized systems composed of particles of a broad range of particle sizes. The degree of particle size heterogeneity determines geometric and micromechanical properties of packings which in turn strongly affects its mechanical response to external loads during shearing [1] and compaction [2] as well as flowing behavior of particle mixtures during discharge processes [3]. Spatial rearrangement of spheres changes both, the number and distribution of contacts in particulate system. In a truly disordered monodisperse packing of spherical frictionless and cohesionless particles, it is expected that the coordination number (*CN*) equals twice the number of degrees of freedom per particle. Thus, it is expected that coordination number in two dimensions is four, whereas in three dimensions it reaches value of six [4]. The packings with such value of *CN* reach mechanical stability and they are called isostatic, while those with higher coordination number are hyperstatic. The latter ones have more contacts than are needed for mechanical stability. For frictional packings, at the jamming transition, spheres can attain contact numbers between d+1 and 2d, where d is a dimension [5]. Contrary to frictionless hard monodisperse spheres which form isostatic packings regardless of construction history and restitution coefficient, frictional packings achieve a multitude of hyperstatic packings and depend on construction history and restitution coefficient. The coordination number decreases smoothly from six with increasing coefficient of friction between two particles which disagrees with the isostaticity hypothesis [6]. The one assumes immediate decrease in coordination number to four as the friction coefficient is increased.

Microstructure characterization of polydisperse particulate media which is critical to understand and predict macroscopic properties of granulate systems, includes basic geometrical and topological parameters such as packing density, void-size distribution, the number of contact, spatial arrangement of contact normals et al.. The packing density of particulate system was reported to be sensitive to both, the particle size heterogeneity as well as percentage contribution of particles of various dimensions [7]. The degree of size dispersity determines packing fraction, the average coordination number, the radial distribution function, and the contact angle distribution [2]. Bentham et al. [2] observed a decrease in average number of contacts and increase in the range of the average number of contacts with the increase in degree of particle size polydispersity in samples composed of microcrystalline cellulose or sucrose.

As the experimental methods do not provide essential knowledge on micromechanical properties of particulate assemblies, theoretical and computational approaches are increasingly preferred to represent granular media. The numerous models have been proposed to simulate packing of polydisperse particles in both 2D and 3D systems [80, 9]. The simulations of packing structure of spherical and spheroidal particles with three types of size distribution performed by Hwang et al. [10] revealed a high influence of type of distribution on packing porosity and average coordination number in system. The increase in standard deviation in normal size distribution resulted in decrease in average coordination number and evolution of distribution of coordination number from normal to asymmetric. The degree of particle size heterogeneity was found to have a high influence on the mechanism of transmission of contact forces in 2D granular system [11]. Increase in particle size heterogeneity results in transformation of disorder from the one where contribution of small particles to the total number of spheres in assembly does not determine packing properties to the one where pore-filling small particles prevails. The decrease in fabric anisotropy was observed with extending particle size distribution. The discrete element simulations of isotropic deformation of frictionless packings of spheres, conducted by Göncü et al. [12], showed that at the same void fraction pressure in system decreases with particle size heterogeneity increasing. The authors have also found that transition from jammed to unjammed state occured at lower void fractions for more polydisperse, heterogeneous packings. Shaebani et al. [13] reported an increase in deviation of the trace of fabric and stress tensors from the average packing properties with increasing degree of particle size polydispersity.

The frictional properties of particles in granular plant materials which are determined by moisture content of grains highly affect packing structure, stiffness and transmission of pressure in particulate media [14, 15]. Wiacek and Molenda [15] observed nearly twofold increase in coefficient of static friction between rapeseed grains with moisture content of grains increasing from 7.5% to 12%. The change of mechanical properties of rapeseed decreased values of effective elastic modulus and pressure ratio of samples under compressive load of 50 kPa by above 20% in both, experimental and numerical tests.

The review of previous studies has shown a high dependence of mechanical properties of granular assembly on both the degree of its polydispersity and interparticle friction. The more insight into that relationship is required to explain and predict the behavior of particulate assemblies under various conditions.

In this paper, the influence of degree of particle size heterogeneity on mechanical response of block shaped specimen composed of frictional and frictionless spheres under compressive loading was studied using discrete element method.

2 MODEL DESCRIPTION

Discrete element method (DEM), based on a microstructural approach [16], is a common numerical technique for detailed investigation of mechanical behavior of granular systems. The simplified non-linear Hertz-Mindlin contact model [17] with elastic spring and viscous damper in the normal direction and spring, damper and frictional slider in the tangential direction were used. 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 calculating normal and tangential contact forces at each incremental time step, which is set small to allow one to assume a constancy of 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 tangential contact force is limited by the Coulomb friction law assuming that particles slide over each other when the tangential force is at limiting friction.

In this study, three-dimensional DEM simulations were conducted using the EDEM software. The mixtures of 1200 spheres polydisperse in size were poured into a steel chamber of rectangular cross-section 0.12 m wide, 0.12 m high and 0.033 m thick (see Fig. 1). Diameter of basic sphere was equal to 7.3 mm. The normal particle size distribution with various standard deviation of particle mean diameter *(SD)* ranging from 0% to 80% was applied. The thickness of sample was recommended as a representative elementary volume in uniaxial compression confined test of monodisperse granular material [18]. The input parameters for the granules [19] and the steel [20] are listed in Table 1.

At first stage of simulation chamber was filled with particles randomly generated in the whole volume of the box. The granules settled down onto the bottom of box under gravitational force. The initial configurations of monodisperse and polydisperse samples with standard deviation of particle mean diameter of 80% are presented in Figure 1. The top lid of box was moved down with constant velocity of $3x10^3$ mm min^{-1} at second stage of simulation until the normal lid pressure reached 100 kPa. Three replications were performed for each value of standard deviation of particle mean diameter.

Table 1: DEM input parameters [17, 18]

<table>
<tr><td>Parameter</td><td colspan="2">Particle</td><td>Steel</td></tr>
<tr><td>Poisson's ratio</td><td colspan="2">0.26</td><td>0.3</td></tr>
<tr><td>Shear modulus (MPa)</td><td colspan="2">560</td><td>200000</td></tr>
<tr><td>Density (kg/m^3)</td><td colspan="2">1720</td><td>7800</td></tr>
<tr><td rowspan="2">Coefficient of restitution</td><td colspan="2">pea-pea</td><td>pea-steel</td></tr>
<tr><td colspan="2">0.21</td><td>0.54</td></tr>
<tr><td rowspan="2">Coefficient of static friction</td><td colspan="2">pea-pea</td><td>pea-steel</td></tr>
<tr><td>0</td><td>0.4</td><td>0.29</td></tr>
<tr><td rowspan="2">Coefficient of rolling friction</td><td colspan="2">pea-pea</td><td>pea-steel</td></tr>
<tr><td colspan="2">0.01</td><td>0.01</td></tr>
</table>

(a) (b)

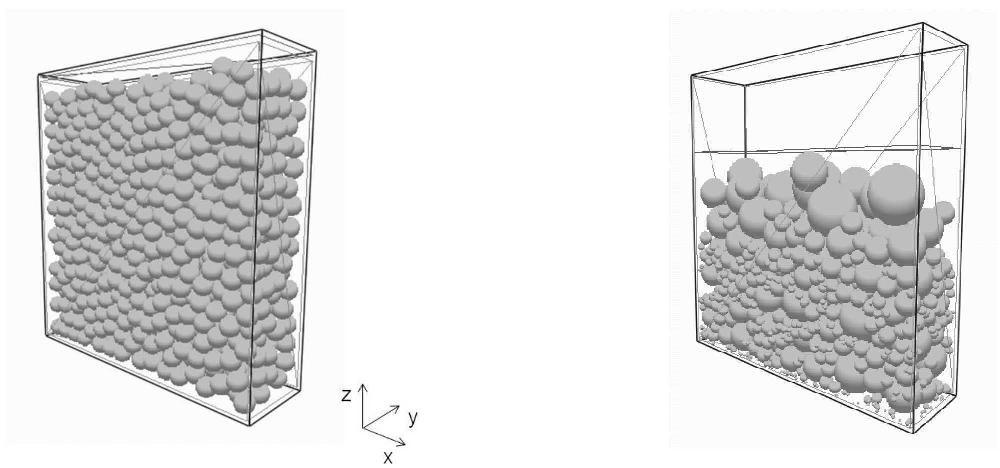

Figure 1: Initial configurations of monodisperse sample (a) and polydisperse sample with standard deviation of particle mean diameter of 80% (b)

3 RESULTS

3.1 Micromechanical characteristics

The discrete element simulations provided the detailed information on the fabric and micromechanical properties of polydisperse granular material subjected to uniaxial compression. The analyses of microstructure of particulate assemblies included the solid fraction, number of contacts and contact forces.

Figure 2 shows the change in solid fraction of particulate assemblies with various degree of polydispersity in samples under vertical loads (σ_v) 100 kPa. The mean values with the error bars indicating ± one standard deviation are shown. The solid fraction is defined as a ratio between the volume of particles in particulate system and its total volume. The slight increase in solid fraction was observed for standard deviation of particle mean diameter increasing up to 50%. Presence of unfilled or partially filled pores between large particles in assemblies of higher degree of particle size heterogeneity decreased solid fraction. The comparison between solid fractions calculated for samples composed of smooth and rough spheres showed about 10% decrease in value of parameter in frictional sphere packings.

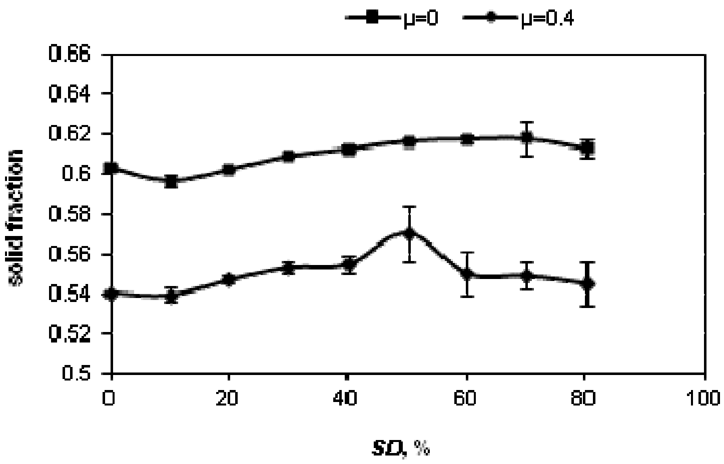

Figure 2: Solid fraction as a function of the standard deviation of particle mean diameter in frictionless and frictional sphere packings at vertical pressure of 100 kPa

The coordination number calculated for mixtures in initial state (before compression) and after compression decreased with *SD* increasing. Uniform spheres in monodisperse samples can get into crystalline formation which leads to homogeneous distribution of contacts is system. Each particle is supported by neighboring particles and it supports few other particles. At low values of *SD* particulate system is characterized by property called long-ranged order in which remote portions of the sample exhibit correlated behavior. Increase in degree of disorder of granules and participation of small particles in mixtures at higher *SD* leads to decrease in total number of contacts and short range order. As the small spheres fill partially the pores left by larger particles, each particle is supported by neighboring particles but it does not necessarily support the other ones. Figure 3 presents evolution of average coordination number with increasing degree of particle size polydispersity at compressive loads of 0 kPa and 100 kPa. The coordination number varied from 4.88 to 1.89 and from 3.91 to 3.16 in frictionless and frictional sphere packings in initial state, respectively. Increase in vertical load to 100kPa increased number of contacts between particles in sphere packings which resulted in coordination number varying from 5.56 to 2.25 and from 4.23 to 2.60 in assemblies composed of frictional and frictionless particles, respectively. The analysis of number of particles staying in contacts only with other particles (spheres staying in contacts with walls were excluded) showed that 25% of particles had six neighbors and 13% of particles had more neighbors in monodisperse frictionless sphere packings. The presence of interparticle friction decreased number of spheres with six contacts to 14% and reduced number of particles with more neighbors to 6%. Exclusion of particles which stayed in contacts with walls increased average coordination number to 5.3 in frictionless sphere packing, that approached system to isostatic state and to 4.4 in frictional sphere packing.

The distributions of number of contacts per particle (N) in uncompressed samples are shown in Fig. 4. The distribution of number of contacts resembles a normal distribution for *SD* of 0% and 20% while for spheres with higher standard deviation of particle mean diameter it became asymmetric and left-skewed. The increase in coefficient of interparticle friction decreased frequency of spheres with five or more neighbors and majority of particles stayed in contact with four or less neighbors.

(a) (b)

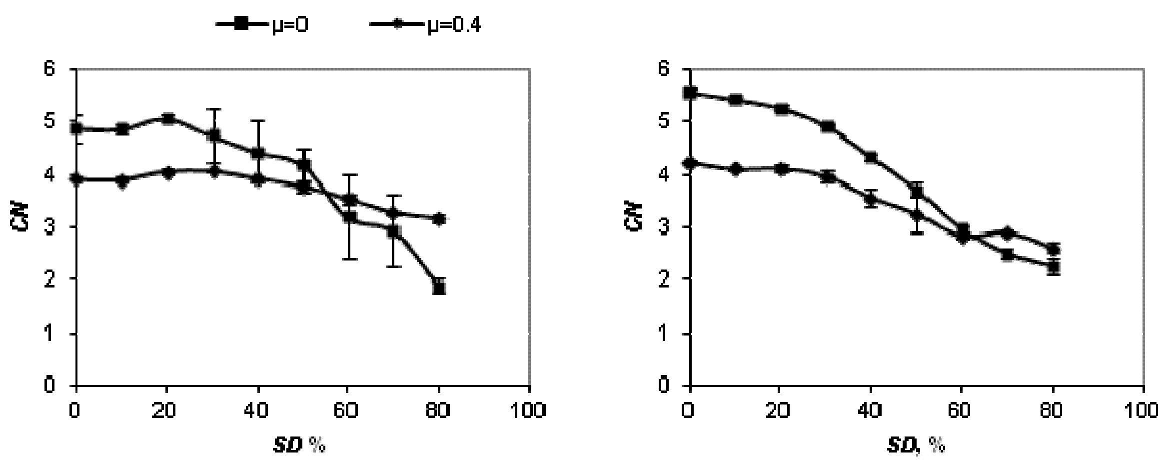

Figure 3: Coordination number as a function of the standard deviation of particle mean diameter in frictionless and frictional sphere packings at vertical pressure of 0 kPa (a) and 100 kPa (b)

The evolution of probability density functions of normal contact forces (F_n) in samples of various particle size polydispersity at vertical pressures of 0 kPa are presented in Fig. 5. The distributions of normal contact forces are asymmetric and left-skewed. The highest inhomogeneity in contact forces in monodisperse systems was observed. The differences between distributions of normal contact forces in frictionless and frictional sphere packings decreased with increase in standard deviation of particle mean diameter.

(a) (b)

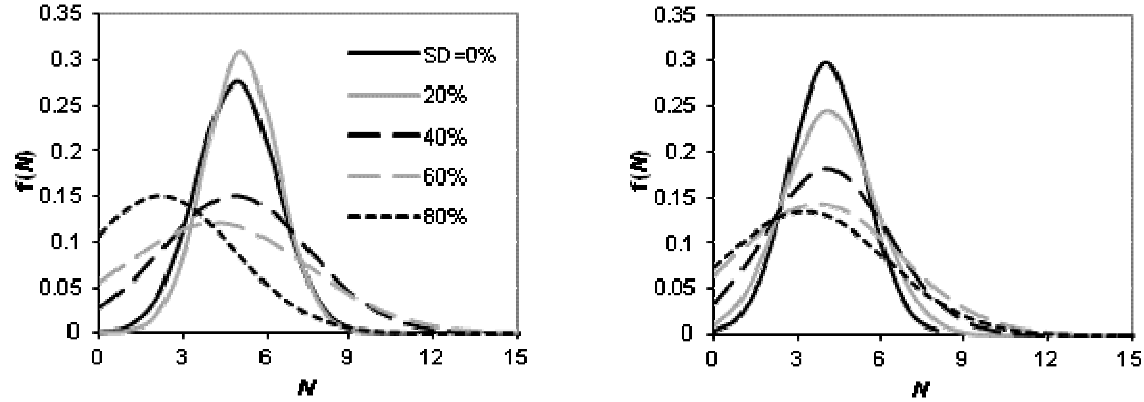

Figure 4: Probability distribution function of number of contacts between particles for various standard deviations of particle mean diameter in frictionless (a) and frictional (b) sphere packings at vertical pressure of 0 kPa

(a) (b)

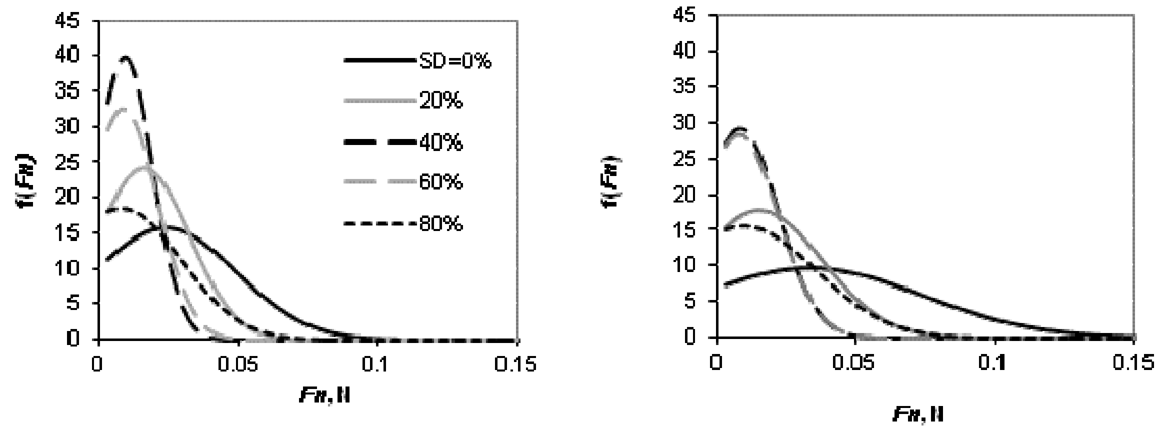

Figure 5: Probability distribution function of normal contact forces for various standard deviations of particle mean diameter in frictionless (a) and frictional (b) sphere packings at vertical pressure of 0 kPa

3.2 Macromechanical characteristics

The study of macromechanical response of polydisperse spherical granular material under compression included the effective elastic modulus, pressure ratio and internal friction angle. The effective elastic modulus *E* which characterizes the bedding elasticity [19] was expressed as follows:

$$E = H\frac{\Delta\sigma_v}{\Delta v}\left(1 - \frac{2k_L^{\ 2}}{1 + k_L^{\ 2}}\right) \tag{1}$$

where H is the height of the assembly, $\Delta\sigma_v$ is the change in vertical pressure during each time step, Δv is change in vertical displacement and k_L is a ratio of change in lateral pressure to change in vertical pressure during each time step. The stiffness of samples with various standard deviations of particle mean diameter increased with compressive loads increasing, however high fluctuations of value of effective elastic modulus in assemblies composed of smooth spheres were observed. Fig. 6 shows the evolution of E value with degree of particle size heterogeneity at vertical pressure of 100 kPa in frictionless and frictional sphere packings. The effective elastic modulus increased with *SD* value increasing up to 50% in sample composed of smooth particles that decreased slightly for higher *SD* values. Effective elastic modulus varied slightly with *SD* values increasing in frictional sphere packings. High variation of E values was observed probably as a result of nonreplicable spatial structure of the assembly. Differences between E value calculated for smooth and rough spheres for *SD* values higher than 30% lied within the range of scatter.

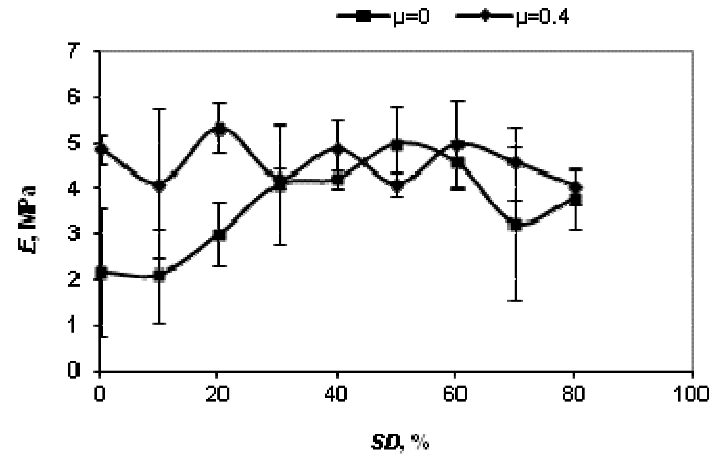

Figure 6: Evolution of effective elastic modulus in samples of various standard deviations of particle mean diameter in frictionless and frictional sphere packings at vertical pressure of 100 kPa

The lateral-to-vertical pressure ratio (k) which is defined as the ratio of the horizontal stress in x direction (see Fig. 1) to the vertical stress was calculated for samples of various standard deviations of particle mean diameter. The evolutions of pressure ratios with *SD* values in frictionless and frictional sphere packings under load of 100 kPa are illustrated in Fig. 7. The discrete element simulations predicted value of pressure ratio of 0.74 for uniform smooth spheres that exponentially decreased to 0.35 in mixture with *SD* of 50%. Increase in standard deviation of particle mean diameter to 80% increased k value to 0.44. Increase in coefficient of interparticle friction resulted in about 40% decrease in pressure ratio, however no change of the direction of evolution of k value with *SD* value increasing was observed.

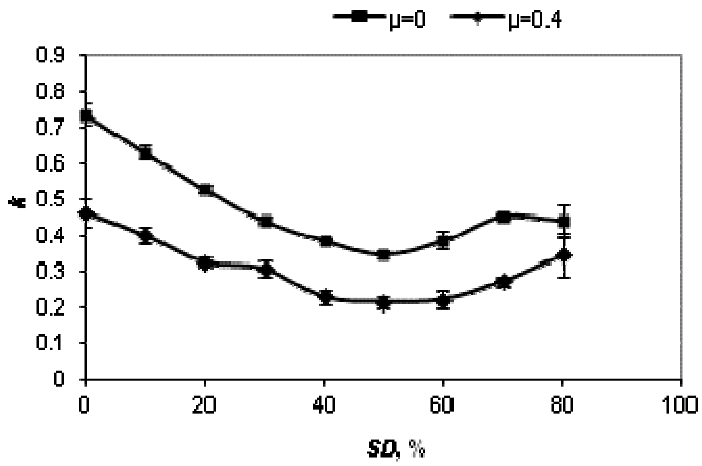

Figure 7: Evolution of lateral-to-vertical pressure ratio in samples of various standard deviations of particle mean diameter in frictionless and frictional sphere packings at vertical pressure of 100 kPa

The values of pressure ratio in granular assemblies were strongly related to values of the angle of internal friction (φ) which highly increased in sphere packings with standard deviations of particle mean diameter increasing up to 50%. Further increase in *SD* value resulted in decrease in φ values. The relationship between pressure ratio and internal friction angle may be expressed by the following formula recommended by[19]:

$$k_\varphi = 1.1(1 - \sin\varphi). \tag{2}$$

The evolutions of angle of internal friction with *SD* values in frictionless and frictional sphere packings under load of 100 kPa are illustrated in Fig. 8.

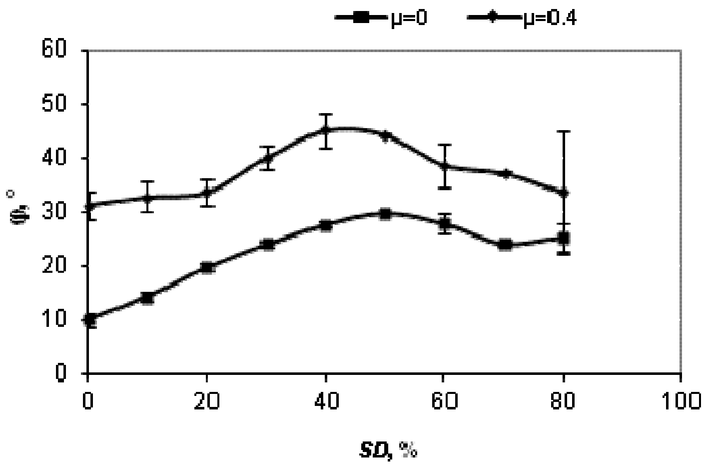

Figure 8: Evolution of the angle of internal friction in samples of various standard deviations of particle mean diameter in frictionless and frictional sphere packings at vertical pressure of 100 kPa

4 CONCLUSIONS

The 3D DEM simulations were conducted with packings composed of frictionless and frictional non-uniformly sized spheres to examine the influence of particle size heterogeneity and interparticle friction on the mechanical properties of a granular assembly under uniaxial compression. The standard deviation of particle mean diameter ranged from 0% to 80%. The micro-scale analyses included distribution of contact forces and average coordination number, whereas macromechanical study included the stress transmission, angle of internal friction and elasticity of the particulate assemblies.

The slight increase in solid fraction was observed for standard deviation of particle mean diameter increasing up to 50%. Further increase in particle size heterogeneity decreased volume of particles due to higher influence of large granules on the fabric of system. The comparison between solid fractions calculated for samples composed of smooth and rough spheres showed about 10% decrease in value of parameter in frictional sphere packings.

The number of contacts decreased with standard deviation of particle mean diameter increasing in both, frictionless and frictional sphere packings. The exclusion of particles which stayed with contacts with walls from analysis of coordination number showed 8% and 12% increase in average coordination number in monodisperse frictionless and frictional sphere packings, respectively. The average coordination number in frictionless sphere packing increased to 5.3, that approached system to isostatic state.

The distributions of normal contact forces between particles in modeled samples were asymmetric and left-skewed. The differences between distributions of normal contact forces in frictionless and frictional sphere packings decreased with increase in standard deviation of particle mean diameter.

The study on influence of degree of polydispersity of granular packings on their stiffness showed increase in effective elastic modulus with *SD* value increasing up to 50% in sample composed of smooth particles that decreased for higher *SD* values. Effective elastic modulus varied slightly with *SD* values increasing in frictional sphere packings. Differences between *E* values calculated for smooth and rough spheres were significant for *SD* values lower than 30%. The differences lied within the range of scatter in samples with higher particle size polydispersity. The degree of particle size heterogeneity in granular assembly was found to determine distribution of pressures in system that resulted in exponential decrease in the lateral-to-vertical pressure ratio in frictionless and frictional sphere packings with standard deviation of particle mean diameter increasing to 50%. After minimum value of lateral-to-vertical pressure ratio was reached, increase in value of parameter was observed with standard deviation of particle mean diameter increasing. Increase in coefficient of interparticle friction from 0 to 0.4 resulted in about 40% decrease in pressure ratio.

The study has shown that degree of dispersity in diameters of particles in granular assembly strongly affects its mechanical response to externally applied stress, which is related to structure and microscopic properties of particulate packing. It was also showed that interparticle friction does not determine direction of change of mechanical parameters with degree of particle size heterogeneity increasing. As the most realistic granular materials involved in industrial and natural processes are characterized by some degree of polydispersity, the scientific outcomes from this project should find wide application to particulate solids.

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