Deformability of polydisperse granular materials: the effect of size span and shape of grain size distribution

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Abstract. This paper investigates the effect of the grain size distribution (GSD) on deformability of spherical particle assemblies using the distinct element method. The GSD is modeled by a normalized beta function, which allows variation of the size span (nearly monodisperse to highly polydisperse) and the shape (approximately linear to strongly curved) of GSD. A series of triaxial compression tests is simulated on a set of assemblies with varying GSDs under different packing fractions and confining pressures. The compressibility under isotropic loading and deformation modulus during shearing are examined for various GSDs. The results show that the size span and shape of GSDs affect the packing conditions of the assemblies but have negligible influence on the compressibility and deformation modulus of the assemblies under the same packing conditions. A unique correlation is found between the deformation modulus and the mechanical coordination number, which can be estimated from the effective void ratio.

1. Introduction

Deformability of granular materials is a significant issue in many earthworks (e.g., rockfill dams). It highly depends on the gain-scale characteristics of particles (e.g., particle size and shape) that constitute the materials [1,2] in addition to the confining pressure, packing fraction, and loading path. In recent decades, progressively increasing research on granular materials has focused on the relationship between the grain-scale attributes and their macroscopic response. One of the most salient issues is the effect of the size polydispersity of a granular aggregate (i.e., consisting of grains of different sizes) on its bulk properties. The majority of investigations has been dedicated to tackling the effect of the polydispersity on packing fraction [3,4] and shear strength [5,6]. For instance, both physical experiment [7] and numerical simulation [3,4] suggested that a broad grain size distribution (GSD), i.e., with larger uniformity coefficient $C_u$, leads to a dense packing due to small pore-filling particles. Several numerical simulations showed that the shear strength of assemblies consisting frictionless or frictional grains, was independent of the size span and shape of GSD in the steady state [5,8]. However, the effect of size polydispersity on the deformability of granular materials is short of studies, and contradictory results emerge from some numerical simulations. For example, [9] suggested that the shape of GSD has little effect on the stiffness of granular materials whereas our previous results [10] showed that highly-truncated GSD clearly influenced the deformation modulus of
granular assemblies. Additional efforts are warranted to improve the fundamental understanding of the grain-size dependence (or independence) of deformability of granular assemblies.

This paper aims at a systematic study on the effect of size polydispersity (characterized by the span and shape of GSD) on the deformation behavior of granular aggregates using the distinct element method (DEM) [11]. A normalized \( \beta \) function [3] is introduced to vary the size span (nearly monodisperse to highly polydisperse) and the shape (approximately linear to pronouncedly curved) of GSD. The deformation modulus of the assemblies is determined from DEM simulations of triaxial compression tests. To eliminate influences from other grain-scale properties (i.e., shape, crush resistance of grains), the particles under consideration are idealized as un-crushable spheres in this preliminary phase. Nevertheless, combined effects of size polydispersity, grain shape, and breakage can be introduced successively in future studies. In this paper, attempts are also made to seek microscopic variables that govern deformation behavior of granular assemblies as GSD varies.

2. DEM simulation

To systematically investigate size polydispersity, we carefully adopt a procedure to prepare samples with progressively varying configurations of GSDs. The size span \( s \) of the distribution is defined as 
\[
s = \frac{(d_{\text{max}} - d_{\text{min}})}{(d_{\text{max}} + d_{\text{min}})},
\]
where \( d_{\text{max}} \) and \( d_{\text{min}} \) are the maximum and minimum particle diameters, respectively; \( s = 0 \) corresponds to a monodisperse distribution, whereas \( s = 1 \) corresponds to an infinitely polydisperse system. This study selects three values of \( s \): 0.40, 0.54, and 0.89. To model the shape of the GSD curve, we employ a normalized \( \beta \) function [3] formulated as follows:
\[
\beta(x) = \frac{1}{B(a,b)} \int_0^x t^{a-1} (1-t)^{b-1} dt
\]
where \( a > 0 \) and \( b > 0 \) control the shape of the distribution; \( B(a,b) = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)} \), where \( \Gamma(\cdot) \) is the Gamma function. The GSD of granular materials frequently confronted in the practice of earthworks is then described as the following cumulative distribution function:
\[
P(d) = \beta \left( x = d_r(d); a, b \right) \times 100\%
\]
where \( P(d) \) is the percentage in mass of particles finer than \( d \); \( d_r(d) = (d - d_{\text{min}})/(d_{\text{max}} - d_{\text{min}}) \) is the reduced diameter. According to [3], this model allows for approximating various GSDs typically occurring in soils (e.g., linear, power-law, and S-shaped distributions) by varying the values of \( s \), \( a \), and \( b \).

In the given simulations, \( a \) is fixed at 2 and \( b \) varies from 0.1 (a hyperbolic distribution in the semilog representation) to 4 (an S-shaped distribution in the same coordinate frame) apart from \( s = 0.89 \). The value of \( b \) for \( s = 0.89 \) is fixed at 0.5 due to the limitation of the total number of particles and hence, the computational cost. We vary \( s \) and \( b \) while arbitrarily setting \( d_{\text{min}} = 3 \) mm and \( a = 2 \), considering that (1) it is primarily the relative size (not the absolute size) that affects the simulation results, and (2) adjusting \( s \) and \( b \) results in sufficient grading variations needed in the simulations. Figure 1 presents eleven GSDs under consideration. Each curve with its own \( C_u \) in parentheses is named by \( s \) value followed by \( b \) value. For instance, \( s0.40_{b0.1} \) indicates that \( s = 0.40 \) and \( b = 0.1 \). The generated GSD within DEM is also exhibited in figure 1 and it coincides with the corresponding theoretical one.

This study uses the open-source DEM simulator YADE [12], which adopts the classical linear elastic-plastic contact law for particles [11]. Although simpler than Hertz-Mindlin formulation [13], the linear model is sufficiently accurate and computationally efficient for the particles at small deformations [14]. The normal contact stiffness \( (K_n) \) and the tangential contact stiffness \( (K_s) \) are computed as follows:
\[
\begin{align*}
K_n &= 2 \frac{ER_iR_z}{(R_i + R_z)} \\
K_s &= \alpha K_n
\end{align*}
\]
where $R_1$ and $R_2$ are particle radii; $E$ is the Young's modulus of the particles, and $\alpha$ is the ratio of tangential to normal stiffnesses. The Coulomb's law is employed to limit the maximum shear force, and the Cundall's non-viscous damping [15] is used to dissipate kinematic energy. Table 1 lists the major parameters taken from typical ranges of common granular materials.

![Image](image_url)

**Figure 1.** Theoretical GSDs (dash lines with symbols) for different combinations of parameters $s$ and $b$, and an example of generated GSD (solid line) in DEM.

| Parameter                   | Value   |
|-----------------------------|---------|
| Particle density (kg/m$^3$) | 2,650   |
| Inter-particle friction $\mu$ | 0.7     |
| Young's modulus $E$ (GPa)   | 1       |
| Particle stiffness ratio $\alpha$ | 0.7   |
| Damping coefficient         | 0.2     |

The DEM simulation is performed under gravity-free conditions in two steps: sample preparation and triaxial compression loading. The gravity-free conditions are set to eliminate the effect of gravity-induced inhomogeneity [16]. Although different from the normal gravity conditions in laboratory, the non-gravity environments in all simulations provide a fair comparison between the results from samples with various GSDs. The conclusions drawn from these simulations are, therefore, referentially valuable for granular materials under the normal gravity conditions in laboratory. During sample preparation, a total of 10,000 (for $s = 0.40, 0.54$) or 24,000 (for $s = 0.89$) dispersed spheres, are randomly generated according to a prescribed GSD within a cubical periodic cell. The total number of particles is limited due to the prohibitive computational cost. Nevertheless, the ratio of the sample size to the maximum particle size is far more than 5, the minimum recommended value to avoid significant size effect of the specimen. The resulting aggregate is then isotropically compressed at 10 kPa using the servo-control algorithm [17]. The aggregate is compressed to two states: loose and dense states, which are used in a relative sense here. To obtain a loose sample, the inter-particle friction coefficient is set to 1.0, and particle rotations are switched off until the mean stress reaches 90% of the target value. Then, the inter-particle friction coefficient is changed to 0.7 and particle rotations are switched on. Based on the loose sample, a dense sample is then attained by altering the inter-particle friction coefficient to 0 and maintaining 10 kPa confining pressure, and eventually resetting the inter-particle friction coefficient to 0.7. When the ratio of the maximum unbalance force to the mean contact force is smaller than a pre-defined tolerance (i.e., $10^{-3}$ according to [4]), we assume that the system reaches force equilibrium and the sample preparation phase ends. Figure 2 shows two DEM samples at different densities for the GSD $s 0.89 \_b 0.5$.

The drained triaxial compression simulation encompasses an isotropic compression phase followed by a shear loading phase. Every sample is isotropically compressed in a stress-controlled manner using the servo-control algorithm under a confining pressure ranging from 300 to 900 kPa until force equilibrium is reached. Afterwards, the aggregate is vertically loaded by moving the top and bottom walls at a constant strain rate of $0.04 \text{ s}^{-1}$. This loading rate is set to ensure that the resulting inertia number given by [18] is no more than $10^{-3}$, indicating quasi-static conditions. Meanwhile, the confining pressure on the side boundaries (i.e., $\sigma^3$) is maintained constant by a servo-control algorithm.
Figure 2. Examples of DEM specimens with different densities: (a) loose specimen; (b) dense specimen for the GSD $s = 0.89$, $b = 0.5$.

3. Results

3.1. Gradings and compressibility

Figure 3 shows the void ratios ($e$) of the samples against the confining pressures ($p$) at the end of isotropic compression stage. For samples under similar packing conditions, the location of the $e$-$p$ curves (i.e., the packing fraction of samples) is notably dependent on both the size span and the shape of GSD. It can be observed that the packing fraction rigorously increases (i.e., the $e$-$p$ curve shifts down) with increasing size span regardless of the shape of the GSD. Despite non-monotonic relation between the packing fraction and shape of GSD, the packing fraction roughly increases monotonically with $C_u$ from all GSDs in this study, which is in good agreement with reported data [4,7].

In addition to the packing fraction, the capability of resisting compaction (i.e., the slope of the $e$-$p$ curve) is also a significant property for granular materials. As illustrated in figure 3, the $e$-$p$ curves of samples at a similar relative density, are nearly parallel to each other despite different size polydispersity; compared to the loose samples, those of dense samples are apparently flatter. It indicates that the spherical granular aggregate at a higher relative density, exhibits higher resistance to compaction, and its compressibility is negligibly influenced by the size polydispersity under consideration.

Figure 3. Compressibility of samples at (a) loose and (b) dense states under isotropic compression.

3.2. Stress-strain response and deformation modulus

Figure 4 and figure 5 show the stress-strain curves respectively obtained from the loose and the dense samples with various GSDs under different confining pressures. The loose and the dense samples exhibit strain-hardening and strain-softening behavior, respectively. From samples at a specific relative density, negligible differences between the stress-strain responses, especially in the elastic stage, are observed, which implies that the deformation behavior of spherical granular aggregates may be independent of the size polydispersity. To quantify this effect, we examine the value of the...
deformation modulus $E_{50}$, defined as the secant slope on the stress-strain curve when the deviatoric stress reaches half of the peak, to quantify the deformation of the aggregates. Figure 6 presents the values of deformation modulus $E_{50}$ from samples with various GSDs as a function of the confining pressure ($\sigma_3$) and grouped by the relative density. $E_{50}$ approximately increases linearly with $\sigma_3$ and the increasing rate of dense samples is apparently lower than that of loose samples. It indicates that the deformation modulus of loose aggregates is more sensitive to confining pressure than that of dense aggregates. As also shown in figure 6, from samples at a similar relative density under a certain confining pressure, the data for the deformation modulus $E_{50}$ roughly converge to a narrow range regardless of GSD. The results confirm that the deformation modulus $E_{50}$ is not sensitive to both the size span and shape of the GSD.

**Figure 4.** The stress-strain responses from loose samples with various GSDs: (a) $b = 0.5$; (b) $s = 0.54$.

**Figure 5.** The stress-strain responses from dense samples with various GSDs: (a) $b = 0.5$; (b) $s = 0.54$.

**Figure 6.** The relationship between the deformation modulus ($E_{50}$) and confining pressure ($\sigma_3$) for samples with various GSDs at different states: (a) loose state; (b) dense state. The symbols are data and the dash lines only a guide to the eye.
3.3. Correlation between deformation modulus and microscopic variable

The prominent impact of the initial loading conditions (packing density and confining pressure) of the granular sample on the deformation modulus $E_{50}$ is shown in figure 6. The pressure and density-dependent bulk properties, such as deformability of granular aggregates, are apparent, and well consistent with laboratory observations. However, the observations from laboratory tests are phenomenological. We wonder about the existence of microscopic properties that intrinsically control the deformability of the aggregates. To explore the macro and microscopic relations, we attempt to correlate $E_{50}$ with the mechanical coordination number ($CN$) [17] of the aggregates at the end of isotropic compression stages. As illustrated in figure 7, the data collapse in a narrow band, implying that $CN$ could succeed in uniquely determining $E_{50}$ at the particle level for the grain-size conditions considered in this study.

![Figure 7. The relationship between the deformation modulus ($E_{50}$) and coordination number ($CN$) for various GSDs at different relative densities.](image)

The relation presented in figure 7 could be useful in practice if $CN$ (which cannot be easily quantified in laboratory) can be estimated from conventionally measurable variables. Figure 8 shows an attempt of linking $CN$ with the void ratio $e$, and the effective void ratio $e'$, excluding particles with less than two contacts (i.e., rattlers without contributing to the loading frame formed by solid particles [19]). $CN$ is well correlated with $e'$ under a certain range of the size polydispersity.

![Figure 8. Coordination number ($CN$) against (a) the void ratio ($e$) and (b) the effective void ratio ($e'$).](image)

4. Conclusions

This study systematically investigates with DEM, the effect of the size polydispersity (characterized by both size span and shape of GSD) on the deformation of aggregates consisting of spherical particles. The numerical samples are first isotropically compressed and then sheared in a triaxial configuration. The simulations successfully capture the main mechanical features of the aggregates at different densities. The results of the study confirm that the packing fraction increases rigorously with the size span and roughly with the uniformity coefficient ($C_u$). The compressibility under isotropic loading and deformation modulus $E_{50}$ during shearing, are examined for various GSDs. The results show negligible differences in the deformation parameters among different GSDs, which indicates that the
deformability of spherical granular assemblies under similar packing conditions is insensitive to the size polydispersity. At the microscale, a unique correlation is found between the deformation modulus of the aggregates and the mechanical $CN$ regardless of variation in size polydispersity. Although practically unmeasurable, the $CN$ can be related to the effective void ratio.

We note that the GSDs studied here have a value of $C_v$ smaller than 2 due to the limit of the particle number and hence the computational cost, whereas in practice, $C_v$ could be substantially larger. Further work is warranted to explore the grain-size dependent behavior of granular materials within a wider range of $C_v$.

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