

EFFECTS OF INTERGRANULAR FRICTION AND GRAIN SIZE DISTRIBUTIONS ON THE INITIAL VOID RATIO OF GRANULAR SAMPLE

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Abstract

This paper investigates the influence of intergranular friction and grain size distributions on the initial void ratio of a granular sample subjected to isotropic compression loading. In the field of geomechanics, besides the loading path and evolution of microscopic properties, the initial void ratio is a crucial and key factor that governs the mechanical behavior of geomaterials. By using Discrete Element Model (DEM) performed on an idealized 2D assembly of disks, this study demonstrates that the initial void ratio can be affected by several parameters during isotropic compression stage. By varying a wide range of intergranular coefficients of friction and grain size distributions, our numerical results suggest that increasing the intergranular coefficient of friction during the isotropic compression phase leads to looser samples. Furthermore, when the diversity of grain sizes is rich, smaller grains can move and occupy voids, thereby increasing the density of the granular sample. A power-law relationship is then proposed that connects the minimum void ratio and the diversity degree of the sample.

Keywords: DEM; Granular materials; sample generation; isotropic compression; initial void ratio; intergranular coefficient of friction; grains size.

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1. Introduction

Granular materials in civil engineering, such as granular soil or sand, exhibit highly complex behavior. Their behavior is not only dependent on the loading path and microscopic changes but also heavily reliant on the initial state of the material. Among them, the initial void ratio is a crucial factor that governs the mechanical response of granular materials under loading. It is well known that the initial compacting level of a granular sample affects the shear strength of the material [1–7]. In more detail, Desrues and co-workers [1, 2] performed a series of biaxial and triaxial tests on dense and loose Hostun sand specimens and showed that their mechanical behavior including strain localization occurrence is affected by the initial void ratio of the sample. This effect was also recognized by [3, 4] when predicting the undrained shear strength of sand-silt mixture and granular soil. The initial state was further explored in terms of particle size gradation and the influence of fine contents on the mechanical strength of granular soils by both experimental and numerical research [5–7]. Moreover, regarding volumetric strain evolution, when subjected to biaxial or triaxial loading, loose samples undergo a unique contracting phase, while denser samples experience a contracting phase followed by a dilating phase before reaching the same critical state. The overall behavior of the granular material is directly reflected by its structure.

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Modeling the behavior of granular materials is to reflect their physical and mechanical characteristics in an overall response. Several approaches have been proposed in the literature for this purpose, including the Finite Element Method (FEM), Discrete Element Method (DEM), Smoothed-particle hydrodynamics (SPH), or coupling with other methods [8–13]. Since its first application in the 1970s, DEM has become a powerful tool for investigating the behavior of granular materials, mainly due to its ability to represent their discrete nature. Although various improvements have been proposed to realistically describe the shape of grains, circular grains (in 2D) and spheres (in 3D) are still the most popular shapes used for modeling granular materials by DEM. The combination of circular or spherical grains with friction and/or rolling resistance can partially meet the requirements of modeling granular materials with real grain shapes [14]. In such cases, a real granular sample is approximated by an idealized medium.

When using DEM to predict the behavior of granular material, sample preparation is an important task. It is not just about correctly reproducing the grain size distribution, but also about describing the initial state, such as the initial void ratio. The initial void ratio of a granular sample can be affected by several factors during the sample preparation process. One of the significant factors is the intergranular friction level, which prevents the sliding of one grain over another, leading to the appearance of more voids within the granular sample. Besides, the grain size distribution is also an important factor. Small grains can easily move and occupy voids between larger grains, thus increasing the compacting level of the granular sample.

Attention has been paid to predicting the maximum and minimum void ratio of granular assemblies by theoretical, numerical, and experimental attempts. In 2002, Cubrinovski and Ishihara [15] conducted an extensive statistical analysis of several types of sand for evaluating their maximum and minimum void ratio. The results showed an important contribution of grain size distribution on the void ratio characteristic of sand. Chang et al. [16] developed an analytical model for predicting the minimum void ratio of granular soil. This model is based on particle gradation curves. Regarding numerical approaches, [17] used DEM (PFC code) for investigating the initial void ratio of the sample. They used particle dumping method to explore the effects of shape, and aspect ratio of grain on the minimum and maximum void ratios of two-dimensional granular assembly. They also showed that the intergranular coefficient of friction can affect the maximum and minimum void ratio. More recently, Sarkar et al. [18] assess the effects of particle and specific gravity characteristics on the extreme values of the initial void ratio. In summary, all these recent works have demonstrated the influence of friction and particle size on the maximum and minimum void ratio. However, these works only focus on the granular sample in the mixture phase and have not considered the influence of such parameters during sample preparation by isotropic compression which is well-known as one of the most popular laboratory tests in the field of geomaterials and an essential task prior to the biaxial or triaxial test.

To shed light on these points and to reveal the microscopic origin of void formation within the granular assembly during isotropic compression tests, this paper aims to investigate the impact of intergranular friction (measured by the coefficient of friction) and grain size (expressed as the ratio between the maximum and minimum grain radius) on the initial void ratio of granular samples. To achieve this goal, we conducted a series of isotropic compression tests using the DEM method, which is commonly used in geomechanics. The remainder of this paper is structured as follows: Section 2 provides an overview of the DEM methodology and sample preparation procedures. Section 3 presents the results and discussion of our study. Finally, we conclude our findings and provide remarks in Section 4.

2. Methodology and numerical samples

In this current research, we use an in-house DEM code developed by Combe and co-authors [19–21] to simulate the behavior of granular materials. The material is idealized by an assembly of circular grains similar to other DEM works [3, 22]. Grains interact via normal elastic force $f_n = k_n \cdot \delta$ and Coulomb friction threshold $f_t \leq \mu \cdot |f_n|$ when they are in contact [20, 23]. In these equations, f_n , f_t are normal and tangential contact force, k_n is normal contact stiffness, δ is the overlapping of two grains in contact, and μ is the intergranular coefficient of friction. We limit to purely frictional granular materials (no bonding at contact point) without rolling resistance. DEM computation is mainly carried out in two steps: first contact forces are computed by the contact model as described just above and then we apply Newton's second law for time integration. A classic third-order predictor-corrector scheme [24] is used.

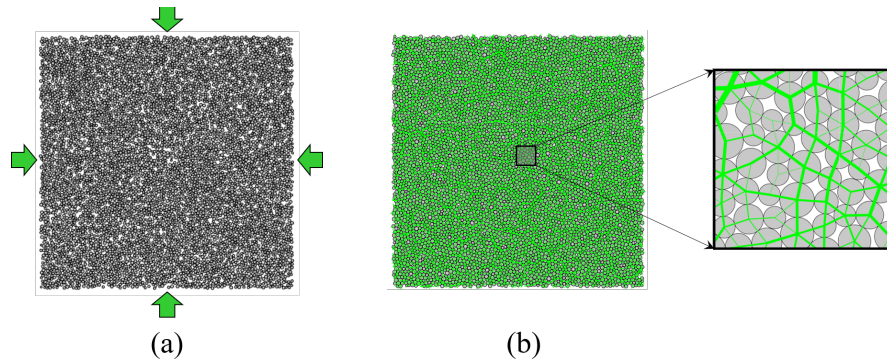


Figure 1. Isotropic compression test by DEM: (a) initial state and (b) sample at the end of isotropic compression with zoom inside the sample (green lines represent the contact pair by joining the center of two grains that interact. The width of the line is proportional to the amplitude of interaction force)

Among laboratory tests, isotropic compression is a very popular one. This can help to estimate the compressive strength of geomaterials or serve as a preparation test for further biaxial or triaxial loading. Thus the quality of the sample after the isotropic compression stage is an essential issue. In this paper, isotropic compression tests were performed to investigate the influence of intergranular friction and particle size distribution on the density of granular packing. To this matter, the granular sample was prepared with a height-to-width ratio of one, following the procedure as described in [20]. The numerical sample was then compressed through four edges with periodic boundary conditions (PBC). The use of PBC was demonstrated to efficiently reduce the number of grains used in the simulation and avoid noise when interacting with rigid walls [9, 25]. The principle of the isotropic compression test is illustrated in Fig. 1. The pressure applied on the four boundary edges was implemented thanks to a stress-controlled procedure. The sample was gradually compressed from the initial state (a) until it reached an equilibrium quasi-static state (b), with intergranular voids reducing as grains interacted with each other.

In this study, we prepared fifteen numerical samples divided into five groups (cases), with each group consisting of three realizations. All samples were composed of 6400 grains with a uniform grain size distribution which is limited by a minimum r_{\min} and maximum r_{\max} grain radius. Five grain-size distributions were used, named case 1 ($r_{\max}/r_{\min} = 0.50/0.10$), case 2 ($r_{\max}/r_{\min} = 0.50/0.15$), case 3 ($r_{\max}/r_{\min} = 0.50/0.20$), case 4 ($r_{\max}/r_{\min} = 0.50/0.25$), and case 5 ($r_{\max}/r_{\min} = 0.50/0.3$). Fig. 2 displays the grain size curves for all five cases. In each case, high similarity in terms of grain size curve is obtained for three realizations of each case. We then perform an isotropic compression test with a certain value of contact friction. In order to investigate the influence of the intergranular coefficient of

friction (μ) on void ratio, we vary μ from 0.0 to 1.0 by step of 0.1, thus $\mu = [0.0 \ 0.1 \ 0.2 \ \dots \ 0.9 \ 1.0]$. A total of $11 \times 3 \times 5 = 165$ simulations have been performed. The computing time for each realization within the same group is similar and varies mainly with the intergranular coefficient of friction used in the simulations. The total running time of approximately 500 hours on a single core of Xeon CPU E5-2680 2.40 Ghz was recorded.

3. Numerical results: what affects void ratio?

In this section, we present simulation results from a series of isotropic compression tests and discuss how the intergranular coefficient of friction and particle size distribution influence the void ratio of the granular sample.

3.1. Effect of intergranular friction

We first explore the influence of μ . Void ratio ($e = V_v/V_s$) is defined as the ratio of the volume of voids (V_v) to the volume of solids (V_s). Fig. 3 displays the initial void ratio (e) of the granular sample after isotropic compression for all considered numerical experiments (red lines). Each sub-figure presents the average line of three realizations for each grain size distribution, along with the error bar which delimits minimum and maximum values of the void ratio over three realizations. Firstly, we observe that the variation of the void ratio is small between realizations of the same group. Secondly, all sub-figures in Fig. 3 follow a similar trend: the initial void ratio of the granular assembly increases with increasing the intergranular coefficient of friction (μ) during isotropic compression, indicating a denser sample is obtained with a smaller value μ . The influence of the friction coefficient during the isotropic compression test on the void ratio is significant in a range of $\mu = [0.0 - 0.5]$. When μ exceeds 0.5, the influence becomes moderate. As μ increases, the rate of void ratio decreases considerably. In contrast to the void ratio, coordination number, defined as the average contact per grain, decreases with increasing of μ during the isotropic compression process (blue lines). Like the void ratio, the influence of μ on the coordination number is more noticeable when μ less than 0.5. Beyond this value, coordination number variation versus μ appears stable in all grain size distribution cases. This observation is easy to understand by linking the coordination number with the void ratio [26]. In fact, as the void ratio increases, more intergranular voids are created, and grains have more space to move. Therefore, they have more opportunities to not be directly in contact with one or several neighboring grains, which reduces both the local and overall number of contacts. The result reported in this paper agrees with several samples which were prepared for 2D DEM investigation of granular material found in the literature. [27] obtains a dense sample $e = 0.21$ with a weak grain-size dispersity. [28, 29] point out that the initial void ratio of dense and loose 2D granular samples is about 0.18 and 0.24, respectively.

We now take a closer look inside the granular sample. At the contact point, when two grains are in contact, they interact via normal and tangential forces. The normal force is considered as elastic behavior while tangential force is of elasto-plastic type with Coulomb threshold. When the tangential force reaches the Coulomb threshold (maximum value), sliding contact occurs. By increasing the intergranular friction, the occurrence of sliding contacts can be prevented. As a result, it becomes

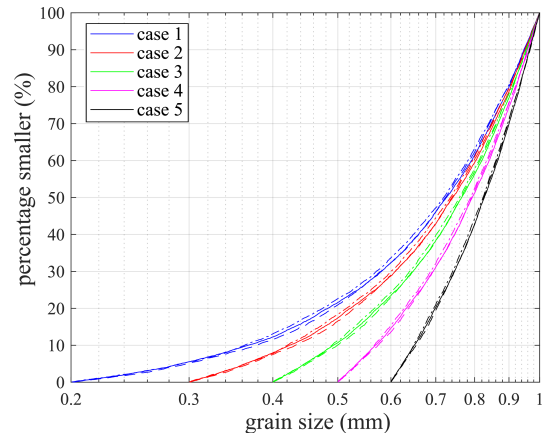


Figure 2. Grain size curves

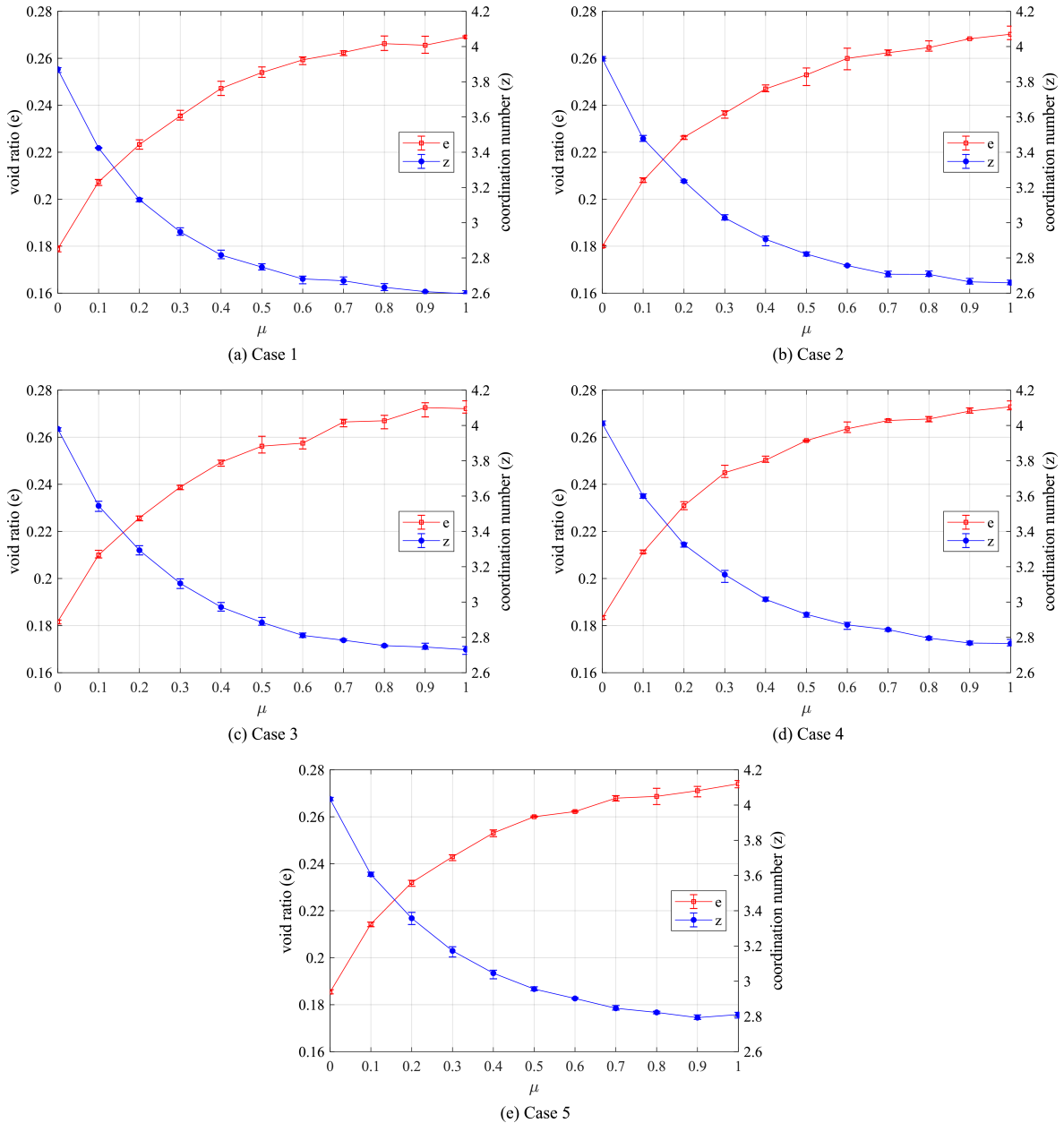


Figure 3. Initial void ratio (e) and coordination number (z) in function of intergranular coefficient of friction for all particle size cases

more difficult for the grains to rotate and create local intergranular voids. The evolution of void ratio (e) along the isotropic loading is shown in Fig. 4(a), where it rapidly decreases to reach the expected value, and then the sample is allowed to relax to reach an equilibrium state. In Fig. 4(b), the coordination number (z) is plotted against the simulation iteration (it). As the sample is compressed, the free grains move to form contact with neighboring grains, causing the total number of contacts and coordination number to increase. Similar to the evolution of the void ratio, the coordination number increases rapidly to reach a plateau. Finally, Fig. 4(c) shows the rate of sliding contacts (compared to the total number of contacts) over simulation time.

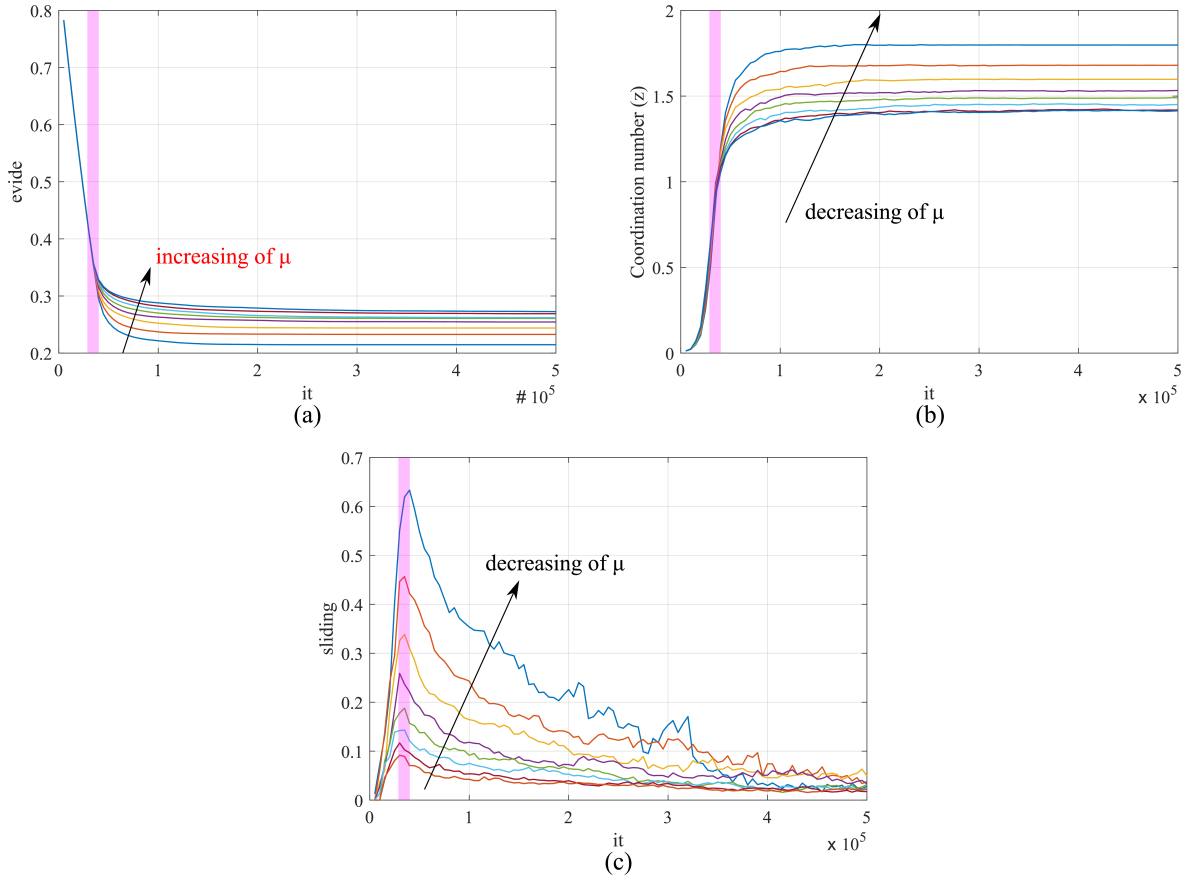


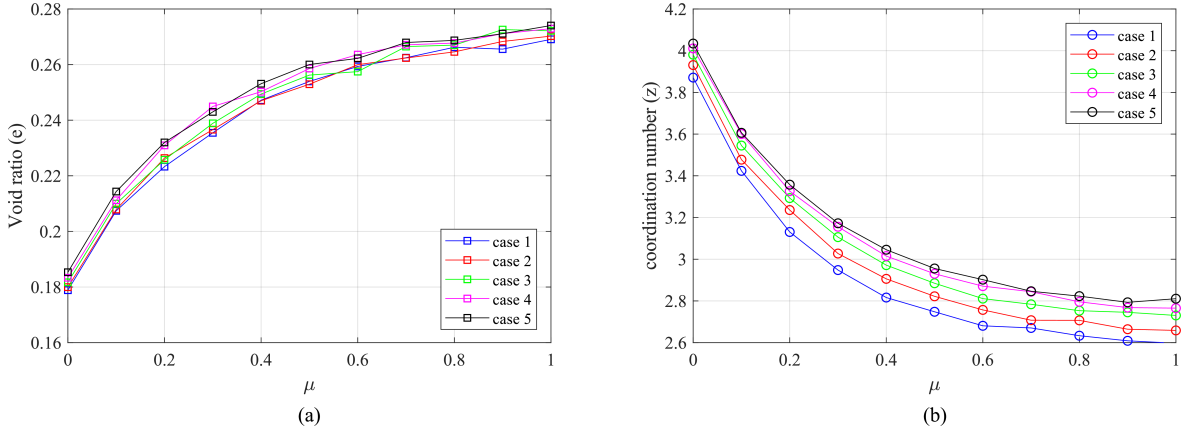
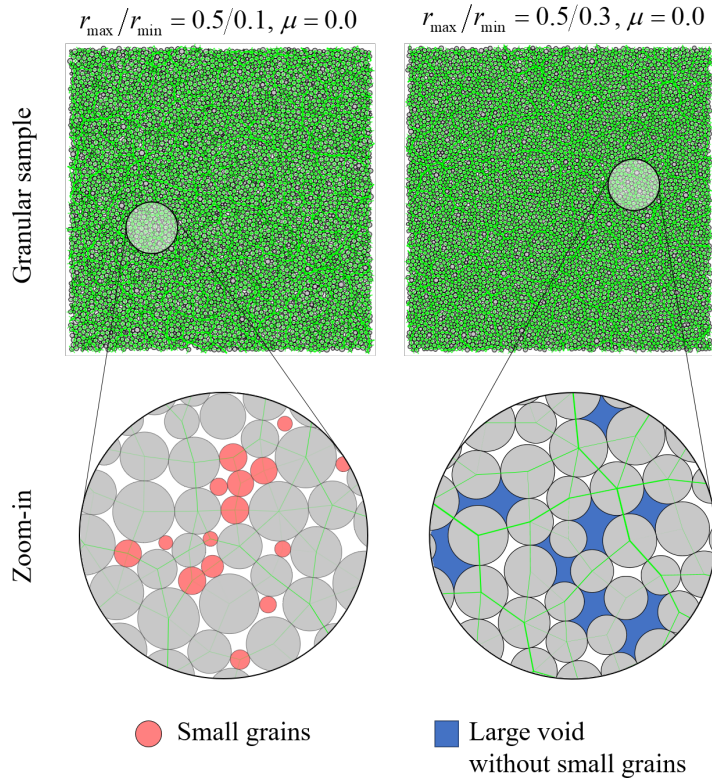
Figure 4. Evolution of the number of sliding contacts and void ratio during isotropic compression.
Typical results extracted from case 5

The results show that the rate of the number of sliding contacts (Fig. 4(c)) increases as the inter-granular coefficient of friction decreases, which is consistent with the reduction in Coulomb threshold $\mu \cdot |f_n|$. During the simulation, all sliding contact rate curves show a peak in the initial phase before entering the descending period. The peaks do not fall in the same iteration point but within a small range, which is delimited by light pink rectangular (hereafter called peak-zone). This narrow zone is placed in two other sub-figures (Fig. 4(a, b)) for comparison. Notably, before passing the peak-zone, the evolutions in void ratio and coordination number are almost identical. Soon after the peak-zone, curves start to diverge to different final values. These consistent observations between the three sub-figures confirm that just after the peak-zones, grains almost find their final positions, and the isotropic stress level is almost reached. The stage up to this point is the most essential one in the isotropic compression process. The rest of the simulation which consumes largely computation time is devoted to system equilibrium in dissipation of grains' kinematic energy.

3.2. Effect of particle size distributions

In Fig. 5, we consider only the average values of each group and report the void ratio and the coordination number in function of the friction coefficient. These two sub-figures show interesting observations.

In this simulation, we kept the maximum grain radius constant while varying the minimum grain size to investigate the effects of particle size distribution on void ratio. As the ratio of small to large


 Figure 5. Average void ratio (e) and coordination number (z)

 Figure 6. Zoom in granular samples (result from case 1 and case 5 with $\mu = 0.0$)

particles (r_{\max}/r_{\min}) increases, there are more small particles present in the granular sample. These small grains can easily move and occupy the intergranular voids between the larger grains, leading to a reduction in the amount of free void space and an increase in the initial density of the sample. This observation is consistent with experimental/theoretical/numerical findings obtained by [16, 30–32]. This phenomenon is observed across the entire range of friction coefficients μ . These observations are further supported by zooming into the sample at the end of isotropic compression loading, as shown in Fig. 6. In the case with a higher ratio of small to large particles $r_{\max}/r_{\min} = 0.5/0.1$, it is clear that smaller grains fill the spaces between larger grains, while in the case with a lower ratio $r_{\max}/r_{\min} = 0.5/0.3$, large intergranular voids without smaller grains are present. As a result, the

overall void ratio of the sample increases. This effect is observed across all cases, regardless of the value of the intergranular coefficient of friction. However, it is evident that a smaller coefficient of friction leads to less local void ratio formation, and small grains have less opportunity to occupy free void space.

It is worth noting that in Fig. 5, the void ratio does not purely increase with decreasing the dispersity in grain size distribution (i.e. r_{\max}/r_{\min}). In fact, it is true for $\mu \leq 0.2$ but when μ is larger, the void ratio of higher r_{\max}/r_{\min} case falls below the one of small r_{\max}/r_{\min} case. This is because the “separate effect” of grain size distribution is no longer advantageous. Instead, we observed a combined effect of both intergranular friction and grain size distribution on void ratio. In particular, when $\mu \leq 0.2$, the effect of intergranular friction dominates but it is no longer valid after exceeding 0.2. Conversely, in terms of the coordination number evolution, for the whole range of μ , the higher dispersity of the sample is, the higher the resulting coordination number is obtained.

3.3. Minimum void ratio of granular sample

In geotechnical practice, the minimum void ratio of granular soil is an important factor that affects shear strength, volume changes, and interstitial fluid conductivity. As the granular soil is composed of grains of various sizes, this property is dependent on grain size distribution [2, 15], and predicting the minimum void ratio is an essential task in theoretical, numerical, and experimental studies [15–18, 33]. In our case, as shown in Fig. 7, the minimum void ratio is obtained with the minimum value of intergranular coefficient of friction ($\mu = 0.0$) in isotropic compression loading. Consistent with experimental observations, this value is grain size distribution dependent and the minimum void ratio is inversely proportional to the grain size dispersity. In the considered range, $e_{\min} = f(\mu)$ seems to fit a power-law relationship.

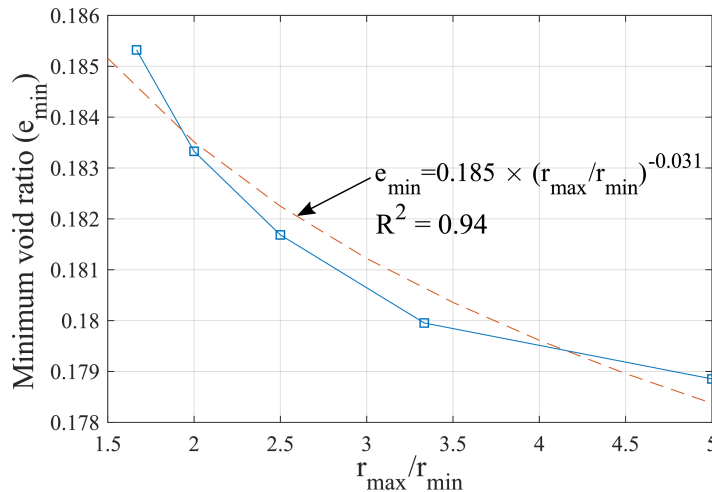


Figure 7. Minimum void ratio versus grain size dispersity ($\mu = 0.0$)

4. Conclusions

In this paper, DEM was employed to investigate the role of the intergranular coefficient of friction and particle size distributions to the initial void ratio of the granular sample. A set of 165 isotropic compression simulations was performed on square samples with periodic boundary conditions. By varying the coefficient of intergranular friction (from 0.0 to 1.0) and the maximum to minimum grains size ratio (from 0.5/0.1 to 0.5/0.3), considerable influences of these two parameters on the initial void ratio of granular assembly are observed. Our findings led to the following conclusions

which can be used as a reference when preparing the sample by isotropic compression process for mechanical investigation of granular materials by DEM.

- Increasing the coefficient of intergranular friction systematically increases the void ratio after isotropic compression. This remark is well consistent with a great reduction in the number of sliding contacts recorded when a high coefficient of friction is used.

- Higher grain size dispersity leads to a decrease in the void ratio of the granular assembly, as smaller grains occupy void spaces between larger grains. In contrast, low dispersity leads to larger void areas with no smaller grains to fill them, resulting in an overall increase in void ratio.

- The minimum void ratio of a granular sample can be obtained by conducting isotropic compression tests with zero friction during the sample preparation process. This parameter may be related to the grain size distribution of the sample, following a power-law relationship.

Although interesting observations have been discussed, our current paper still has limitations. The works should be extended for the case with rolling resistance. Rolling resistance is expected to contribute to the inhibition of free rotation thus changing the density of the granular sample. Additionally, the behavior of granular assembly is also affected by the coordination number. This is somewhat shown by several authors [34, 35]. Future research could explore the combined effects of void ratio and coordination number on granular behavior.

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