Influence of particle size distribution on the proportion of stress-transmitting particles and implications for measures of soil state

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Abstract

It is generally accepted that the use of void ratio and bulk density as measures of soil state have limitations in the case of gap-graded soils as the finer grains may not transmit stress. However, hitherto no one has systematically explored whether this issue also emerges for soils with continuous gradings. Building on a number of experimental and discrete element method (DEM) studies that have considered the idea of an effective void ratio for gap-graded or bi-modal soils, this contribution extends consideration of this concept to a broader range of particle size distributions. By exploiting high performance computers, this study considers a range of ideal isotropically compressed samples of spherical particles with linear, fractal and gap-graded (bimodal and trimodal) particle size distributions. The materials’ initial packing densities are controlled by varying the inter-particle coefficient of friction. The results show that even for soils with continuous particle size distributions, a significant proportion of the finer particles may not transmit stress and be inactive. Drawing on ideas put forward in relation to gap-graded soils, both a mechanical void ratio and mechanical bulk density that consider the inactive grains as part of the void space are determined. Even for the linear and fractal gradings considered here, the difference between the conventional measures and the mechanical measures is finite and density dependent. The difference is measurably larger in the looser samples considered. These data highlight a conceptual/fundamental limitation of using the global void ratio as a measure of state in expressions to predict granular material behaviour.

Notation

ρ	bulk density
ρ_m	mechanical bulk density
D^*	fractal dimension
d^p	particle diameter
b	variable that quantifies the relative contribution of finer grains to stress transmission
c	constant parameter in void ratio correction function
C_u	uniformity coefficient
D_{50}	median diameter of the coarser grains
d_{50}	median diameter of the finer grains
DEM	Discrete Element Method
d^p_{max}	maximum particle diameter
d^p_{min}	minimum particle diameter
e	global void ratio
e^*	equivalent void ratio
e_g	intergranular void ratio
e_m	mechanical void ratio,
e_{sk}	skeleton void ratio
$F_{coarser}$	the proportion by mass of coarser grains in the material
F_{finer}	the proportion by mass of finer grains in the material
F_{int}	the proportion by mass of intermediate grains in the material
G	shear stiffness
G_c	specific gravity of coarser grains
G_{equ}	equivalent shear stiffness
G_f	specific gravity of finer grains
G_{zx}	shear stiffness for zx plane
G_{zy}	shear stiffness for zy plane
M	cumulative mass of grains whose particle diameter is smaller than d^p_i
M_T	total mass of specimens
PSD	particle size distribution
S^*	threshold finer fraction
SR	size ratio between coarser and finer grains
V_s	shear wave velocity
Z	coordination number
μ	inter-particle friction coefficients
v	Poisson’s ratio

Introduction

The global void ratio, *e,* and the bulk density, ρ, are measures of the granular material state that are routinely used to interpret data and predict soil behaviour. Considering the conceptual diagrams of soil presented, for example, in undergraduate textbooks, there is an implicit understanding that the particle phase of the soil is engaged in stress transmission and that changes in packing density relate to variations in the way contacting particles are arranged.

When interpreting laboratory geophysics tests the shear wave velocity, V_s, and the small-strain (elastic) shear stiffness, *G*, are related as

$$G = \rho V_s^2 \tag{1}$$

Equation 1 was derived assuming a homogeneous elastic continuum material. Using discrete element method (DEM) simulation data, Nguyen & O'Sullivan (2019) compared dynamic shear stiffness values deduced from simulations of wave propagation tests with static shear stiffness values obtained from stress probes. For the ideal isotropic, monodisperse samples they considered the two stiffness values should agree if equation (1) is valid. However, this agreement was only observed for the denser packing they considered. Experimental verification of equation 1 is non trivial; Lings (2001) showed that the shear stiffnesses deduced from an axial probe in a triaxial cell, G_{equ}, does not directly correspond to either G_{zx} or G_{zy}. Using horizontally mounted piezoceramic shear plates, Dutta (2019) observed experimentally that the extent to which static and dynamic measurements agree seems to depend on the specific material considered.

Various so-called void ratio correction functions (*F(e)*) have been proposed in the literature to describe the expected variation of *G* with packing density. Amongst other expressions *F(e)* may be estimated by equation (2) (Hardin and Black, 1966) or equation (3) (Jamiolkowski et al., 1995).

$$\mathrm{F(e)} = \frac{(\mathrm{c} - \mathrm{e})^2}{1 + \mathrm{e}} \tag{2}$$

$$\mathrm{F(e)} = \mathrm{e}^{\mathrm{d}} \tag{3}$$

where *c* is empirically assessed to be 2.97 for angular silica sands and 2.17 for rounded silica sands. Similarly, *d* is an empirical fitting parameter. These and other expressions documented in the literature are empirical and lack a fundamental mechanical basis. As outlined in Otsubo (2016), effective medium theory, whether adopting a static or kinematic hypothesis, indicates that density effects should be accounted for by considering both *e* and coordination number, *Z*, (i.e. the average number of contacts per particle) (e.g. Chang & Liao, 1994). Similarly, the simulation data in Agnolin & Roux (2007) demonstrate a link between stress wave propagation velocity and coordination number. Based on empirical analysis of stiffness data obtained from discrete element method (DEM) simulations on virtual samples of soil, Nguyen et al. (2018) highlighted the challenge of developing a correction function including *e* and *Z* that can be applied for a range of anisotropic stress states.

While DEM simulations consider ideal model soils, the data generated can include the individual particle stresses and the forces between contacting particles. Consequently, DEM can be used to directly quantify the relative contribution of each particle to stress transmission and so inform understanding of stress transmission in soil. Numerous DEM studies have identified the existence of particles that do not transmit stress (often referred to as rattler particles), and suggested that analysis of the mechanical behaviour should exclude consideration of these particles from the solid phase of the material, e.g. Thornton (2000). Using DEM data, an alternative state variable, the mechanical void ratio, e_m, can be determined (Otsubo, 2016). In the case of gravity-free DEM simulations, this mechanical void ratio is calculated by considering grains with 0 or 1 contact points, which do not transmit stress, to be part of the void volume. Furthermore, fundamental studies of the material stiffness (Yimsiri & Soga, 2000; Otsubo 2016) have indicated that there is a stronger correlation between G and e_m than there is between G and e.

Gap-graded soils are poorly graded soils which have a deficiency of certain particle sizes. The simplest gap-graded soils which are almost bimodal mixtures of non-plastic finer and coarser grains have been considered in studies that have considered the response to shear deformation (e.g. Carraro et al., 2009), resistance to liquefaction (e.g. Thevanayagam et al., 2002), susceptibility to internal instability (e.g. Skempton & Brogan, 1994) and small-strain stiffness (e.g. Yang & Liu, 2016). Restricting consideration to non-plastic finer particles, these prior studies have often focused on the sensitivity of the mechanical behaviour to the proportion (i.e. percentage) by mass of finer grains in the material (F_{finer}).

By systematically increasing F_{finer}, these studies, amongst others, have classified behaviour of soil mixtures based on F_{finer} (e.g. Thevanayagam & Mohan, 2000) considering two categories: (1) coarser grains-dominated behaviour; this occurs when F_{finer} is relatively low; (2) finer grains-dominated behaviour; this occurs when F_{finer} exceeds a certain value. The F_{finer} delineating these two classes of soil mixtures is termed the threshold finer fraction (S^*). However, the identification of S^* remains an unresolved issue. Zuo & Baudet (2015) reviewed existing methods used to determine S^* and found that different, rational methods may give different S^* values. Zuo & Baudet (2015) also proposed that S^* is highly dependent on a size ratio between grain size between coarser and finer grains. Rahman et al. (2014) suggested that the concept of S^* is an idealisation of a transition zone rather than having a unique value.

Using DEM, Shire et al. (2014) and Shire et al. (2016) took the ratio of the average stress in the finer grains to the overall applied stress as an index of the proportion of the overall stress transmitted by finer grains. They showed that the extent to which finer grains participate in stress transmission depends on F_{finer} and on the size ratio $SR = D_{50}/d_{50}$, where D_{50} is the median diameter of the coarser grains, and d_{50} is the median diameter of the finer grains). The data in Shire et al. (2014) do not support the concept of a unique S^*, rather a more gradual transition between coarser- and finer particle-dominated behaviour. They identified three classifications based on F_{finer}: (1) coarser grain dominated; (2) transitional, density dependant, behaviour; (3) finer grain dominated. Shire et al. (2016) studied the effect of *SR* for bimodal soils in a dense condition, which highlighted that stress transmission of gap-graded soils is dependent on both F_{finer} and *SR* simultaneously.

The possibility that some particles might not transmit stress has been explicitly recognised amongst experimental researchers in the case of gap-graded soils. Various state variables have been proposed to replace the conventional global void ratio, *e,* to capture the contribution (or lack of contribution) of finer grains to stress transmission. An intergranular void ratio, e_g, proposed by Mitchell (1976) assumes that only a negligible proportion of the finer grains plays an active role in stress transmission and treats the volume occupied by all of the finer grains as if it were void space, thereby:

$$e_g = \frac{e(G_f - G_f F_{finer} + G_c F_{finer}) + G_c F_{finer}}{G_f(1 - F_{finer})} \tag{4}$$

where G_f and G_c are the specific gravities of the finer and coarser grains, respectively. Assuming that G_f equals G_c, Shen et al. (1977) introduced a skeleton void ratio, e_{sk}:

$$e_{sk} = \frac{e + F_{finer}}{(1 - F_{finer})} \tag{5}$$

However, several studies (e.g. Thevanayagam, 2000; Ni et al., 2005) have indicated that it is inaccurate to assume that the entire finer fraction does not transfer stress. Consequently, an equivalent void ratio, e^* was proposed by Thevanayagam and Sabanayagam (2000):

$$e^* = \frac{e + (1 - b)F_{finer}}{1 - (1 - b)F_{finer}} \tag{6}$$

where *b* is a variable that quantifies the relative contribution of the finer grains to stress transmission. Rahman et al. (2008) proposed a semi-empirical relation to determine this *b* value that considers F_{finer}, S^* and the *SR*.

While some researchers (e.g. Rahman & Lo, 2008) have shown that the use of e^* may enable prediction of the mechanical behaviour of soil mixtures, others (e.g. Carrera et al., 2011; Yang et al., 2015) have indicated that the *b* parameter lacks a physical meaning. In particular, Yang et al. (2015) argued that neither e_{sk} nor e^* are useful; they highlighted the lack of investigations to account for complex particle scale interaction between coarser and finer grains and argued that *e* remains an appropriate state variable for soil mixtures.

Throughout the discussion on effective void ratio, prior research has exclusively considered gap-graded / bimodal mixtures. The current study extends consideration to a broader range of particle size distribution (PSD) shapes to better understand the extent to which this issue is unique to or particularly significant for gap-graded / bimodal soils. In doing so we recognize that naturally geological deposits of purely bimodal soils are rare and so a comprehensive and relevant understanding of stress distribution in soil needs to consider a broader range of particle size distributions. Initially continuous gradings (linear and fractal PSDs) are investigated before considering both bimodal and trimodal gap-graded samples.

Numerical Simulation Approach

The DEM simulations used a modified version of the open-source Molecular Dynamics code Granular LAMMPS (Plimpton, 1995). The cubic samples considered were encased within periodic boundary conditions to minimize boundary effects (e.g. Thornton, 2000; Shire et al., 2014). A simplified Hertz-Mindlin contact model was used. The basic input simulation parameters were the shear modulus of single grain (G = 29.17 GPa), the Poisson's ratio (v = 0.2) and the density of the simulated grains (2670 kg/m^3). These input simulation parameters have been used in previous DEM studies (e.g. Huang, et al., 2014) and are similar to experimentally derived values (e.g. Barreto, 2009). In all cases the grains were initially placed randomly in diffuse (non-contacting) positions by means of an in-house placement code. This code ensures a homogenous distribution of particles, i.e. particles can be placed at any position even if they intersect one of the periodic boundaries. A stress-controlled algorithm was used to adjust the periodic boundaries to achieve isotropic stress of p' = 500 kPa for most of the simulations, adopting the method proposed by Cundall (1988) that is also clarified in Thornton (2000). It was confirmed that the coordination number, Z (the average value of contacts per grain), remained stable (i.e. any variation was less than 0.001) for 500,000 simulation cycles prior to terminating the simulations for data analysis. Moreover, it was confirmed that the unbalanced force ratio was lower than 0.001 at the end of each simulation.

In DEM-based studies the coefficient of friction is often used to control sample density during specimen generation (e.g. Thornton, 2000). Following Shire et al. (2014) and Shire & O'Sullivan (2016), to investigate density effects three inter-particle friction coefficients, μ, were used during isotropic compression: (1) μ = 0.001, which generated "dense" specimens; (2) μ = 0.1, which generated "medium-dense" specimens; and (3) μ = 0.3, which generated "loose" specimens. This approach to specimen generation allows different packing geometries capable of transmitting stress to be generated in a systematic and controlled manner. However, the loose and dense specimens created in this way do not directly correspond to specimens created in the laboratory with relative densities of 0% and 100% respectively. It is not possible to directly map the medium-dense samples to a particular relative density.

Only isotropic samples of spherical particles are considered here. The study is limited as this material is highly ideal, however this approach has enabled isolation of the effect of particle size distribution. Particle shape has a significant effect on granular material packing density (e.g. Cho et al., 2006; Youd, 1973; Zhao et al., 2018; Zhao et al., 2020). The current study focused on spherical particles in order to enable a large number of samples with different PSDs to be considered as simulations with non-spherical particles are computationally more expensive. Consequently the range of attainable void ratios is narrower than is the case for a natural sand with more irregular particle morphologies, e.g. Cho et al. (2006), and varies with sample PSD. There is certainly scope to extend this parametric study in the future to include consideration of particle shape. Artigaut et al. (2019) indicated that fabric anisotropy can affect the proportion of stress that is transmitted by the finer grains in bi-modal materials, so there is also merit in considering fabric effects in future studies. Excluding consideration of shape and fabric a very large database of 201 samples was created as detailed below.

PSDs considered

As illustrated in Figure 1(a), 6 "linear" samples with linear gradings were created where the coefficient of uniformity, C_u, was systematically varied. The minimum particle diameter, d_{min}^p, used in each linear specimen was 0.076 mm and the maximum particle diameter, d_{max}^p, increased with increasing C_u. Four "fractal" specimens with a fractal grading were also considered since it has been proposed that fragments generated by weathering and explosions always satisfy a fractal PSD (Tyler & Wheatcraft, 1992). The fractal specimens (Figure 1(b)) were created based on a fractal model proposed by Tyler & Wheatcraft (1992):

$$\frac{M(d^p < d_i^p)}{M_T} = (\frac{d_i^p}{d_{max}^p})^{3-D^*} \tag{7}$$

where d^p is the particle diameter, $M\ (d^p < d_i^p)$ is the cumulative mass of grains whose particle diameter is smaller than d_i^p, M_T is the total mass of specimens and D^* is the fractal dimension. The grading curves for the fractal specimens are plotted in both semi-logarithmic and double-logarithmic coordinate axes (Figure 1(b)). Two d_{max}^p values (0.425 mm and 0.985 mm) were used to create fractal specimens comparable to the linear specimens. (The fractal sample with the smaller maximum diameter, i.e. d_{max}^p of 0.425 mm is denoted *S*, while the sample with the larger d_{max}^p of 0.985 mm is denoted *L*). Rather than explicitly specifying d_{min}^p, as illustrated in Figure 1(b) the particle diameter of 0.076 mm was associated with both the 0.1% volume percentile and the 1% volume percentile for both values of d_{max}^p considered. The fractal dimensions were estimated by curve fitting Equation (7) to the PSDs, as illustrated in Figure 1(b). For instance, the sample 'Fractal 0.1% L' has a d_{max}^p of 0.985 mm and the diameter of the 0.1% volume percentile is 0.076 mm.

For the bimodal gap-graded specimens four *SR* (D_{50}/d_{50}) values were considered: 3.7, 8.4, 13.0 and 18.1. There was a slight polydispersity in the two fractions within each sample. The d_{min}^p was the same as that used in the linear specimens (i.e. 0.076 mm), while d_{max}^p increased with increasing *SR.* For the "bimodal" specimens, 8 values of F_{finer} were used to systematically study the bimodal mixtures (i.e. 5%, 10%, 15%, 20%, 25%, 30%, 35%, 50%). Typical bimodal particle size distributions are illustrated in Figure 1(c). Each sample is identified by its *SR* and F_{finer}. For instance, 'SR 8.4 $\mathrm{F}_{\mathrm{finer}}$ 35' indicates a bimodal material with *SR* = 8.4 and F_{finer} = 35%. When considering bi-modal, gap-graded soils it is important to consider the size ratio at which the finer particles plausibly can exist unstressed within the void space. Shire et al. (2016) found that while in three dimensions the largest sphere which can fit within the void body of the densest face centered cubic packing of uniform spheres (e = 0.35) occurs at *SR* ≈

4.45, a clear indication of bi-modal behaviour occurs for *SR* values ≥ 6.

For the trimodal specimens, an intermediate volume fraction, F_{int}, was considered in addition to F_{finer} and $F_{coarser}$. The trimodal specimens were created to consider a PSD shape that is more complex than the bimodal cases, while also enabling consideration of the influence of relative particle size on stress transmission. Each trimodal specimen considered had the same d^p_{min} of 0.076 mm, an intermediate grain diameter, d^p_{int}, of 0.425 mm and a d^p_{max} of 0.985 mm. Each sample is identified as Tri A_B, where A represents F_{finer} and B represents F_{int}. For instance, 'Tri 10_60' indicates a trimodal material with F_{finer} of 10% and F_{int} of 60%. Some typical trimodal particle size distributions are illustrated in Figure 1(d).

A total of 201 simulations were completed as summarized in Table 1. To achieve representative element volumes the system size considered depended on the particular PSD of the sample, so that up to 636,871 particles were considered in the simulations; the average number of particles in a simulation was 108,806.

Results and discussion

Linear Specimens

Key data relating to the proportion of stress transmitting particles for the specimens with linear PSDs are presented in Figure 2. Figure 2(a) illustrates the cumulative distribution of the particle connectivity values by the number of particles for the dense samples considered. A particle's connectivity is the number of contacts that it participates in; the average connectivity of a sample equals to *Z*. Samples with no contact or only one contact cannot transmit stress and are considered to be inactive. These data illustrate that, for these linear specimens, a relatively large number of grains have connectivity values of 0 and are not active in stress transmission. The proportion of inactive grains increases with increasing C_u. However, referring to Figure 2(b), which illustrates the cumulative distribution of the particle connectivity values by particle volume the volumetric percentage of inactive grains is much smaller than the percentage by number of inactive grains. For instance, in the dense case, when C_u is 6, approximately 24% of particles by number are inactive. In contrast, for the same specimen, only approximately 4% of particles by volume are inactive. This is because these inactive grains are the smaller grains that occupy a small proportion of the total volume of particles. As illustrated in Figure 3(a) and 3(b), the D_{50} of these inactive grains is approximately 0.088 mm regardless of the C_u, while the D_{50} of the active grains increases with increasing C_u. In addition, Figure 2(b) illustrates that the maximum particle connectivity value significantly increases with increasing C_u.

Figures 2(c) & 2(d) illustrate the influence of packing density on the cumulative distribution of the particle connectivity values for a representative linear sample with C_u = 3.6. The proportion of grains by number that are inactive in stress transmission is clearly density-dependent (Figure 2(c)). In the loose case approximately 45% of the total number of particles do not transfer stress, while approximately 19% of the particles in the densest sample are non-stress-transmitting. While the volumetric proportion of grains that are inactive is smaller than the proportion by number (Figure 2(d)), for the loosest sample considered the volumetric proportion of inactive grains is relatively large (i.e. 13.5%).

Figure 3(c) and (d) compare the variation in the proportion of inactive particles with C_u for all of the linear samples, considering both the proportion by number of particles (Figure 3(c)) and the proportion by particle volume (Figure 3(d)). The proportion by number of inactive grains increases with increasing C_u; there is a less obvious increase in the volumetric proportion of inactive grains with increasing C_u. It is clear that for the ideal scenarios considered here, there is a significant density effect.

Consideration of connectivity and the proportion of inactive grains takes a binary perspective, i.e. the proportion of the contribution made by each of those grains that are actively engaged in stress transmission is not captured.

To ensure that the specimen sizes considered were sufficient to generate representative data for the linear specimens, two specimens were created with the same particle size distribution (C_u of 2.4) but different specimen sizes, i.e. 9,045 grains and 42,896 grains. Figure 4(a) shows that the connectivity data for these two specimens are very similar and Figure 4(b) shows that the proportions of inactive grains calculated by particle number and by volume are very similar at all three packing densities considered. The larger sample size could then reasonably be considered to be representative for the data collation presented here. The number of particles should increase with C_u and so the sample sizes ranged from 33,306 for C_u=1.2 to 147,316 for C_u=6. Developing upon the ideas that have hitherto been put forward for gap-graded soils, Figure 5(a) compares e_m and e for the linear samples. As would be expected the e_m values consistently are larger than the e values. Figure 5(b), which considers the variation in $(e_m-e)/e$ with C_u, shows that the magnitude of this difference is finite relative to e for all the samples considered and relatively large in the case of the looser samples. For C_u values exceeding 2, the difference $(e_m-e)/e$ is less sensitive to variations in C_u than it is to variations in density. Figure 5(c) considers the effect on the calculated sample bulk density by calculating the relative difference $(\rho - \rho_m)/\rho$ where ρ_m is calculated assuming the inactive particles to be part of the void space. Considering the data from this perspective there are also measurable differences, particularly when the loose samples are considered. The data presented in Figure 5 indicate that the extent to which void ratio and bulk density give an accurate representation of the density of stress transmitting grains varies with C_u and density.

Specimens with a fractal grading

Figure 6(a) presents cumulative distributions of the particle connectivities for the fractal samples, while Figure 6(b) is the cumulative distribution of connectivities by particle volume. For all of these fractal specimens considered, a large proportion of the total number of grains has a connectivity value of 0 or 1 and is inactive in stress transmission.

For instance, for Fractal 1% L, more than 90% of the particles are inactive. Note that for these fractal specimens, there are a large number of grains whose diameters are lower than 0.076 mm, these grains are dominantly inactive. Consequently a large number of inactive particles is identified for fractal specimens. The volumetric proportion of inactive particles is lower, but still finite (Figure 6(b)), indicating that it is the smaller particles that are inactive. As illustrated in Figure 6(c) and (d) the D_{50} values of the inactive grains are significantly smaller than those of the active grains.

Referring to Figure 7(a), as was the case for the linear samples, the e_m values for the fractal samples are consistently larger than the e values. Figure 7(b) shows that the relative difference $(e_m-e)/e$ is very large. For instance, for Fractal 1% L, these relative differences are approximately 41% and 70% in the dense and loose condition, respectively. The normalized density difference is also significant and exceeds 16% for one of the loosest cases (Figure 7(c)). While the shapes of the PSDs differ from the linear cases, the data on Figure 7 further demonstrates the limitation of e as a metric that can quantify the proportion of a sample engaged in stress transmission / density of stress transmitting contacts and particles even where the PSD shape is continuous.

Bimodal specimens

For the bimodal specimens, the effect of specimen size on the data generated was investigated for a typical bimodal gradation (i.e. SR 8.4 F_{finer} 25). Two distinct specimen sizes were considered: a larger specimen with 100,871 grains and a smaller specimen with 40,020 grains. In each case three densities were considered. Referring to Figure 8(a), for a given density, the observed cumulative distributions of connectivity values are similar for both samples. Furthermore, the data on Figure 8(b) indicate that proportion of inactive grains are indistinguishable for a given density. Several similar checks were carried out for a number of representative samples (e.g. SR 3.7 F_{finer} 50, SR 13.0 F_{finer} 10). In all cases the data were similar, and the larger sample size was used in the data analysis presented here. Connectivity data for the bimodal samples with two distinct *SRs* (i.e. 3.7; 18.1) are included in Figure 9. For each *SR,* both underfilled samples with F_{finer} = 10% (Figures 9(a) & (c)) and overfilled samples with F_{finer} = 50% (Figures 9(b) & (d)) are shown. The connectivities of the finer and coarser grains as well as the total connectivity values are presented in each cumulative distribution plot.

For each *SR,* when F_{finer} is 10% (Figures 9(a) & (c)), more than 80% of the finer particles have a connectivity value of 0, indicating that almost all of the stress is transmitted by the coarser grains. The maximum connectivity values of these coarser particles are approximately 20. In contrast, when F_{finer} is 50% (Figures 9(b) & (d)), a different picture emerges so that approximately 90% by volume of the finer particles are active in stress transmission. For both *SRs* considered in (Figure 9), packing density has a clear effect - the maximum connectivity value increases from the loose condition to the dense condition. In addition, with increasing *SR*, the maximum and median connectivity values of the particles also increases significantly for all fractions.

For instance, for a *SR* of 3.7, the maximum connectivity value is approximately 70, while the maximum connectivity value increases to approximately 1700 when *SR* increases to 18.1.

As with the linear and the fractal specimens, the two measures of void ratio e and e_m are considered in Figure 10 for all the bimodal specimens. When *SR* is 3.7, a finite difference can be observed for all mixtures, however, when *SR* is equal to or larger than 8.4, packing density has a significant effect when F_{finer} is 25% and 30%. However, when F_{finer} is larger than 35%, the difference between e and e_m becomes small irrespective of density, indicating that these finer particles are active in stress transmission. Furthermore, the variation in e with the coefficient of friction used during isotropic compression is small for $F_{finer} \geq 35\%$.

Figure 11 summarizes the proportions of inactive particles for all the bimodal samples considered here. For the *SR* = 3.7 specimen, the proportion by number of inactive grains (Figure 11(a)) can be as high as 81.1 % (loose specimen with F_{finer} =15%), a higher numerical proportion of inactive grains is also observed in the underfilled sample with *SR* larger than 8.4. In the loose *SR* 18.1 specimen with F_{finer} = 10% (Figure 11(e)), over 99% of the particles have a connectivity value of 0, indicating almost all of the stress is transmitted by the coarser grains.

As illustrated in Figure 11(a), (c) & (e), while the proportion by number of inactive particles is extremely large for the samples with low F_{finer} values, this value decreases significantly with increasing F_{finer}, with the sharpest decrease being observed between F_{finer} = 25% and F_{finer} = 30% in the loose and dense cases. These values are close to the critical F_{finer} as indicated in Skempton & Brogan (1994), which is considered to lie between F_{finer} = 24% and 29% in the dense and loose condition, respectively.

The relationship between the proportion by number of inactive grains and the proportion by volume of inactive grains is non-trivial; the data on Figures 11(b), (d) & (f) show considerably less variation in the volumetric proportion of inactive grains with F_{finer} when compared with the significant variation in the numerical proportion of inactive grains with F_{finer}. As illustrated in Figure 11(d) & (f), the data also suggests that soil fabric may change from a filled fabric to an underfilled fabric when the density is varied. For instance, for *SR* 18.1 F_{finer} 25 in the dense condition, approximately 1% grains by particle volume are inactive. In contrast, in the loose condition, approximately 33% of grains are inactive. This result shows that the inactive grains are finer grains, similar to the case for the linear specimens.

Figure 11 also indicates that there is a clear *SR* effect. Whether you consider the proportion by number or the proportion by volume, for the specimens with *SR* of 3.7, the proportion of inactive grains increases gradually when F_{finer} are relatively low (i.e. F_{finer} < 25%), followed by a smooth decrease when F_{finer} larger than 25%. In contrast, for *SR* values equal to and larger than 8.4, the proportion of inactive grains may significantly drop with increasing F_{finer}. For instance, for the SR of 18.1 in the dense condition, the proportion of inactive grains decreases from 22.7% to 0.62% when F_{finer} changes from 20% to 25%. The difference among these SR values can be explained geometrically; as noted by Shire et al. (2016) consideration of the diameter of the largest sphere which can fit in the void space between uniform spheres in their densest face centered cubic packing gives a SR of 4.45.

While the proportion by volume of inactive grains in the bimodal samples is higher than in the case of the samples with continuous grading (Figure 3), the differences are not always very marked. Referring to Figure 11, when SR = 3.7, the maximum proportion of inactive grains in the loose samples is about 15% which is close to the maximum volumetric proportion of inactive grains in the loose linear and fractal samples. The volumetric proportions of inactive grains for the dense samples with SR = 3.7 are also similar to the data for the dense linear and fractal samples. For the cases with SR larger than 8.4 samples, the volumetric proportion of inactive grains is very small for F_{finer} exceeding 30%. For the sample that is definitely underfilled, the proportions are higher than in the samples that are overfilled, but they are not dramatically higher than in the case of the samples with continuous grading; excluding some outlier samples with F_{finer} = 25% and 30%.

Figure 12 considers the effect on the state variables e and ρ for each SR considered for the bimodal samples. As illustrated in Figure 12(a), (c) & (e), the difference $(e - e_m)/e$ is generally relatively low for the samples with SR = 3.7. This relative difference increases with increasing SR, while showing similar magnitude when SR is equal to or larger than 8.4. However, the differences in bulk density measures are not significantly greater than was observed for the samples with continuous gradings. In the case of the samples with SR values equal to or larger than 8.4, significant differences are observed in the case of the underfilled samples with test F_{finer} = 25% and F_{finer} = 30%. Particularly, when F_{finer} is larger than 35%, this bulk density difference may be smaller than the difference identified from continuous gradings.

As discussed above, different state variables have been proposed to enable prediction of the behaviour of gap-graded soils. In this study, these state variables were also calculated based on the measured global void ratio, e. The b values used in calculating the equivalent void ratio, e^*, followed the empirical equation proposed in Rahman et al. (2008). The SR of 18.1 was considered with F_{finer} being lower than the calculated threshold finer fraction (S^*). In the dense condition, as illustrated in Figure 13(a), similar values can be identified for these different state variables when F_{finer} is 5% and 10% and most of the finer particles are inactive. In contrast, when F_{finer} ranges from 15% and 30%, these proposed state variables start to diverge. The calculated e_{sk} is significantly larger than e_m and e^* because the finer grains are active in the stress transmission in this case. In the medium and loose conditions, even when F_{finer} is 5% and 10%, a finite difference is observed amongst the values of e_m, e^* and e_{sk}. The data also indicate a significant density effect that is not considered in the calculation of e^*

and e_{sk}. In particular, considering the loose samples, the e_m values are larger compared to those of e_{sk} and e^*. This result may be attributed to the fact that not all coarser grains are active in the stress transmission.

Trimodal specimens

Specimen size effects were also investigated for a typical gradation as illustrated for trimodal gradation Tri 10_70 in Figure 14. Key particle-scale data for two specimens are compared: a small specimen with 83,069 grains and a larger specimen with 636,871 grains. Both the distribution of connectivities (Figure 14(a)) and the proportion of inactive particles (Figure 14(b)) are very similar, showing that a sample of approximately 83,069 grains is sufficient to get representative results for this grading. These comparison data, along with the experience gained with the linear and bimodal samples, informed the sample sizes used for the remaining trimodal gradations.

Typical simulation results for samples Tri 10_30 and Tri 10_60 are presented in Figure 15(a) and Figure 15(b), which illustrate cumulative distributions of connectivity by particle number and by volume, respectively. Figure 15(a) indicates that more than 99% of particles by number are inactive in the stress transmission; indicating an underfilled soil fabric. A measurable density effect can be observed for specimens Tri 10_30 and Tri 10_60; for both specimens, the connectivity value of grains observed in the dense condition is slightly larger than the value identified for the medium and loose conditions.

Connectivity distribution data for specimens Tri 25_15 and Tri 25_45 are presented in Figure 15(c) and Figure 15(d), these give the cumulative distributions of connectivity by particle number and by volume, respectively. This result shows that when F_{finer} is 25%, a significant change in the nature of stress transmission can be identified. For instance, in the dense condition, for Tri 25_45, approximately 5% grains by particle number are inactive. In contrast, when referring to the loose condition, more than 98% of particles are inactive.

The two measures of void ratio e and e_m are considered in Figure 16 for the trimodal specimens. When F_{finer} is 10%, a finite difference can be observed for all mixtures, however, packing density has a significant effect when F_{finer} is 20% and 25%. The difference between e and e_m can be significant in the case of the loose samples. When F_{finer} is 30%, the difference between e and e_m reduces as the finer particles become active in stress transmission.

Figure 17 summarizes the relative differences in void ratio and bulk density for the trimodal specimens. As was the case in the bimodal samples at low F_{finer} values (i.e. F_{finer} = 10%) the relative differences in void ratio and bulk density are approximately 120% and 26%, respectively. When F_{finer} is 20% and 25%, a clear density effect is also observed for some samples (e.g. Tri 20_20; Tri 25_45). For instance, for Tri 20_30, the difference in bulk density is approximately 1% in the dense condition. In contrast, a significant difference (i.e. 32 %) can be identified for this Tri 20_30 in the loose condition. The extent to which the observed stress transmission patterns are stress-dependent varies with PSD; for instance, significantly greater density dependence is observed for Tri 25_15 or Tri 25_45 than in the case of Tri 20_10 or Tri 20_70. When F_{finer} is 30%, only small error can be observed, which suggests that these finer particles start to transfer stress despite the density condition. In general, the tendency identified in these specimens suggests that trimodal gap-graded soils are more sensitive to the effect of density than bimodal gap-graded soils.

Conclusions

This paper has presented results from a comprehensive DEM investigation of samples with different types of PSD in order to appraise, at a fundamental level, the extent to which void ratio and bulk density are appropriate measures of material state for non-plastic soils. Use of high-performance computing enabled 201 samples to be created and these samples contained up to 636,871 particles. An in-house specimen generation code ensured the distribution of particles within the sample was not influenced by the periodic boundary locations. The significant idealizations in the modelling approach, namely the spherical particle geometries, the isotropic stress state, and the use of friction to control packing density, have been adopted in a number of prior geomechanics studies using DEM. The study has taken a rather simplistic binary approach, by considering the connectivity and the proportion of inactive grains so that the distribution or variations in the contribution made by the stress-transmitting particles is not considered. There may well be merit in looking at the heterogeneity of stress transmission in the active grains, however significant insight is obtained in the current “binary” study.

The data presented here for isotropic samples of spherical particles have shown that even for continuous PSDs (i.e. linear and fractal specimens), a large number of relatively small grains may not be active in transferring stress. While these inactive grains are small in size, in some cases the proportion of the overall sample volume they occupy is finite so that when they are considered to be part of the void space in order to quantify the material state, there is a finite effect on both void ratio and density. The difference between the void ratio, e, that considers the volume of all grains, and the mechanical void ratio, e_m, that considers only stress transmitting grains in the solid volume, is highly density-dependent. This poses a problem: we know at a fundamental level that stiffness, in particular, is closely correlated to e_m. The accuracy with which we can approximate e_m by considering e varies with density and the difference is most pronounced for loose samples. This must compromise the use of e in empirical expressions to predict soil behaviour.

The shortcomings of using e as a predictor of soil behaviour have long been recognised in relation to gap-graded or bi-modal soils. The current contribution has shown that the range of materials for which e is a poor measure of the state is broader than has hitherto been appreciated. The large discrepancy between e and e_m in the case of loose materials is particularly significant as these materials have the greatest susceptibility to liquefaction. This research indicates that experimental programmes that have explored these issues in gap-graded soils should be extended to a broader range of soils.

Data Availability Statement

Some or all data, models, or code that support the findings of this study are available from the corresponding author upon reasonable request.

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Table 1: Summary of analyses

Specimen type	**Range of system size considered**	**Number of simulations**
Linear	33,306 particles for *Linear* C_u *1.5*; 147,316 particles for *Linear* C_u *6.0*;	18 (3 packing densities x 6 PSDs)
Fractal	59,698 particles for *Fractal 0.1% S*; 102,978 particles for *Fractal 1% L*	12 (3 packing densities x 4 PSDs)
Bimodal	16,968 particles for *SR 8.4* F_{finer} *10* ; 481,611 particles for *SR 18.1* F_{finer} *50*	102 (3 packing densities x 34 PSDs)
Trimodal	83,069 particles for *Tri 10_70 (S)*; 636,871 particles for *Tri 10_70 (L)*	69 (3 packing densities x 23 PSDs)