A micromechanical study of the equivalent granular void ratio of soil mixtures using DEM

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ABSTRACT: The concept of intergranular void ratio has become more popular in characterising the behaviour of soil mixtures of sand and fine particles up to a threshold transitional fines content. The transitional fines content at which these mixtures change from a sand-dominated to a fines-dominated behaviour is usually defined as the densest mixture. For samples having a less-than-transitional fines content, the fine particles can fall inside the void spaces created by the larger sand particles. Assuming all fine particles are inactive and hence treated as void, the compression curves of different sand-dominated mixtures can be represented by a single curve in term of the intergranular void ratio. More recently an additional '*b*' parameter was defined as the fraction of the active fine particles out of the total fine content and only the inactive fine fraction was counted as void. The value of *b* was usually obtained from back-analysis or predicted using a semi-empirical approach. In this numerical study using the Discrete Element Method (DEM), various definitions of the intergranular void ratio *e** are investigated and discussed, together with the micromechanical data showing the actual involvement of the fine particles in the force transmission. The results show that the value of *b* is related to the fraction of the fine particles involved in transmitting the strong, larger-than-average contact forces. The value of *b* is not constant but increases with stress level (decreasing void ratio) and fines content for samples having fines content less than the threshold value.

1 INTRODUCTION

Mixtures of clean sand with finer soil materials were shown to have significantly different behaviour compared to the well-understood behaviour of the host sand and this can pose challenges to geotechnical engineers when they need to assess the stability of these materials. Nocilla et al. (2006) studied the behaviour of well-graded silty soils and found that there were no unique normal compression and critical state lines. Thevanayagam (1998) studied the effect of fine material and of fines content on the undrained shear strength of a host sand and found that adding a small fines content (e.g. 10%) can reduce the steady state strength of the mixtures as compared to the strength of the host sand at the same void ratio and the behaviour of silty sand is more sensitive to the confining stress value. Mitchell (1976) studied the role of fines in a granular structure and introduced the concept of a non-active clay content. To describe the behaviour of a silty sand, Thevanayagam (1998) suggested an equation for the intergranular void ratio where the role of the fine particles that fall inside the void space and do not actively transfer forces can be ignored; these fine particles can be treated as void. The intergranular void ratio was considered to be "an index of active coarser-granular frictional contacts that sustain the normal and shear forces".

Thevanayagam (2000) revised the equation of the intergranular void ratio to take into account a possible fraction of the finer size grains that can participate in the force transmission; the new parameter named equivalent intergranular contact index (or "equivalent granular void ratio" by other authors) can be calculated as follows:

$$e^* = \frac{e + (1-b)\,f_c}{1-(1-b)\,f_c}; \quad 0 \le b \le 1 \tag{1}$$

where f_c is the fines content and b is the fraction of the active fine grains; for b = 0, Eq. 1 becomes the equation of intergranular void ratio. Using Eq. 1 for mixtures of fine contents less than a threshold value (f_{thre}), the normal compression lines (and similarly the critical state lines) of different mixtures can be represented by a common line in a *e*-logp'* space. The application of Eq. 1 is however limited as the value of parameter *b* is generally not known and has to be back-calculated using the experimental data of mixtures of different fines contents. Recently Rahman et al. (2008, 2011) reviewed Eq. 1 and recommended a semi-empirical relationship for the estimation of b and another relationship for the value of f_{thre} as functions of χ, the particle-size ratio between the coarse and fine particles in a mixture as follows:

$$b = \left[1 - \exp\left(-0.3\frac{f_c / f_{thre}}{k}\right)\right] \times \left(r\frac{f_c}{f_{thre}}\right)^r \quad (2)$$

$$f_{thre} = 0.4\left(\frac{1}{1+e^{\alpha-\beta\chi}} + \frac{1}{\chi}\right) \quad (3)$$

where $\chi = 1/r = d_{10}^{sand} / d_{50}^{fine}$; $k = 1 - r^{0.25}$; α=0.5 and β=0.13; d_{10}^{sand} is the particle diameter obtained at the point of 10%-finer on the particle size distribution curve (PSD) of sand material, similarly d_{50}^{fine} is d_{50} of the fine material.

Although the intergranular and equivalent granular void ratios were intended to serve as indexes of the active frictional contacts, they were only idealized concepts and it was not clear how to define the active contacts exactly, so it would be impossible to determine the fraction of the participating fine particles using experimental data in soil mechanics. Using Discrete Element Method (DEM) we were however able to study explicitly the force transmission between particles of different sizes in a mixture system and provide for the first time a microscopic explanation for the conceptual equivalent granular void ratio. The fraction of the active fine particles in term of parameter b is now defined explicitly as the fraction of the fine particles that are involved in the strong forces (the contact forces were found solely attributable to the deviator stress of a granular system).

2 DEM SIMULATION OF GRANULAR MIXTURES

The DEM software package PFC3D (Itasca, 2008) was used to simulate the one dimensional (1D) compression behaviour of mixtures of two component materials: a finer uniform material of 0.1 mm diameter and another coarser material having a sand-like PSD as shown in the inset of Fig. 1. Mixture samples were created using different mixing ratios by mass. Interactions between spherical particles were simulated using a simple linear elastic model (Itasca, 2008) with the particle stiffness defined as a function of the particle diameter as shown in Table 1. For sample preparation, first gas-like particle assemblies having an initial porosity of 0.5 were generated randomly and the samples were brought to an initial mean stress value under isotropic compression and zero gravity. A common DEM sample preparation technique was utilized where a temporary friction value of 0.0 was used in this stage to create dense samples. Particle friction was reset to 0.5 and the granular samples were then compressed vertically by moving the top and bottom walls towards a horizontal mid-plane while the lateral walls were fixed. Isotropic and 1D compression stages were conducted in a strain-controlled manner following the same procedure as described in Minh and Cheng (2010, 2013a). The input parameters for the DEM simulations are given in Table 1.

Table 1. Input parameters for 3D DEM simulations.

Input Parameters	Value
Particle friction, μ	0.5
Elastic contact modulus, E_c	1*10^9 N/m^2
Particle normal stiffness, k_n	$k_n = 4*E_c*R$
Particle stiffness ratio, k_s/k_n	1.0
Wall friction, μ_{wall}	0.0
Wall stiffness, k_{wall}	100*< particle stiffness >

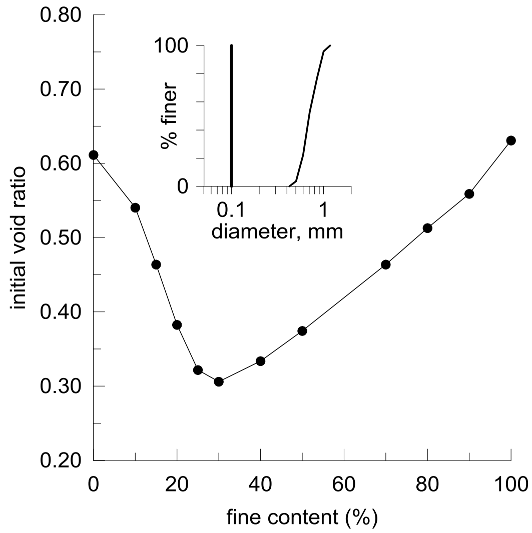

Figure 1. Variation of initial void ratio with fines content; Inset: particle size distribution of the mixing component soils.

Figure 1 shows the variation of the initial void ratio calculated at the beginning of 1D compression for mixtures having different fines content values. A minimum initial void ratio was obtained at approximately 30% fines content, which can be considered as the threshold fines content value in this series of DEM simulations. In another publication (Minh et al. 2014), using the same DEM mixture samples data set we investigated the force transmission at contacts between different particle sizes and concluded that for samples having less than 30% fine contents, the fine particles mostly fall within the void space between coarser sand particles and the contact forces between fine particles do not contribute significantly to the shearing resistance of the whole system. The behaviour of these samples can be classified as sand-particle-dominated. The behaviour of samples having higher than 30% fine contents is dominated by fine particles as evidenced by the fact that as the contact forces between fine particles contribute more significantly to the macroscopic deviator stress, the contribution of the sand-sand particle contact forces decreases and mostly disappears at around 70%-80% fines contents (Minh et al. 2014). According to the definition of the equivalent granular void ratio, e^*, it can be applied to the DEM data in this study for samples of fine contents less than the threshold value of 30%.

Figures 2a and 2b show a natural-scale plot and a semi-log-scale plot of the 1D compression curves of mixture samples in terms of the conventional void ratio, *e*. In both plots, the shape of the curves for fines contents in the range of 10%-20% is similar to each other and similar to the curve for 0% fines, i.e. the pure sand sample. The sample with 30% fines is in the lowest position as it starts from the minimum void ratio value as shown in Fig. 1. The 40% fines sample is shown to represent the behaviour of the group of samples having fines contents higher than the threshold value, which are dominated by fine particles and their compression curves gradually approach the pure sand sample curve at higher fines content values. Although the semi-log plot is more commonly used in soil mechanics to determine the slope of the normal compression line, here the natural scale will be used to plot the curves in terms of intergranular and equivalent granular void ratios in order to discern the differences between the curves more easily.

2.1 *Intergranular and equivalent granular void ratios*

The intergranular void ratio of mixture samples can be calculated using Eq. 1 where *b* is equal to zero, which considers that no fine particle participate in the force transmission; the results are shown in Fig. 3. The curves of 10% fine to 20% fine start from the same initial intergranular void ratio whereas the initial e^* of the 25% fine sample is close to the 10-20% fines cases. Note that all mixture samples have higher initial e^* values than the 0% fines sample, which means that the coarse granular structures of mixtures are looser than for the pure sand sample and hence mixture samples should have been more compressible (if the fine particles do not compensate for this effect). It can be stated that the intergranular void ratio is at most accurate to describe the initial state of the coarse granular structures of mixtures but not the whole compression curves which are significantly different as shown in Fig. 3. The assumption $b = 0$ is more appropriate at low stress range but as the compression process reduces the void space volume, *b* should be larger than zero when the fine particles develop force-transmitting contacts. The change in *b* value should be dependent on the fines content and this explains the deviation of the curves of 10%-20% fines starting from the same initial e^* point.

Rahman et al. (2008, 2011) suggested that Eqs. 2 and 3 can be used to estimate the values of *b* and f_{thre} based on only the size ratio value of the two component materials in a mixture. Applying the equations for our DEM data we get the following results:

$$d_{10}^{sand}=0.53, d_{50}^{fine}=0.1, \chi=d_{10}^{sand}/d_{50}^{fine}=5.3,$$

$r=1/\chi=0.19, k=1-r^{0.25}=0.34$, f_{thre} = 0.29. The values of *b* were calculated for different fines content values and listed in Table 2. Similar to the intergranular void ratio, the *b*-value of the equivalent granular void ratio is a constant, which does not depend on the void ratio or the stress values.

Table 2. *b*-values obtained using the approach by Rahman et al.

Fine content (%)	10	15	20	25	30	40
b-value	0.15	0.23	0.31	0.37	0.43	0.54

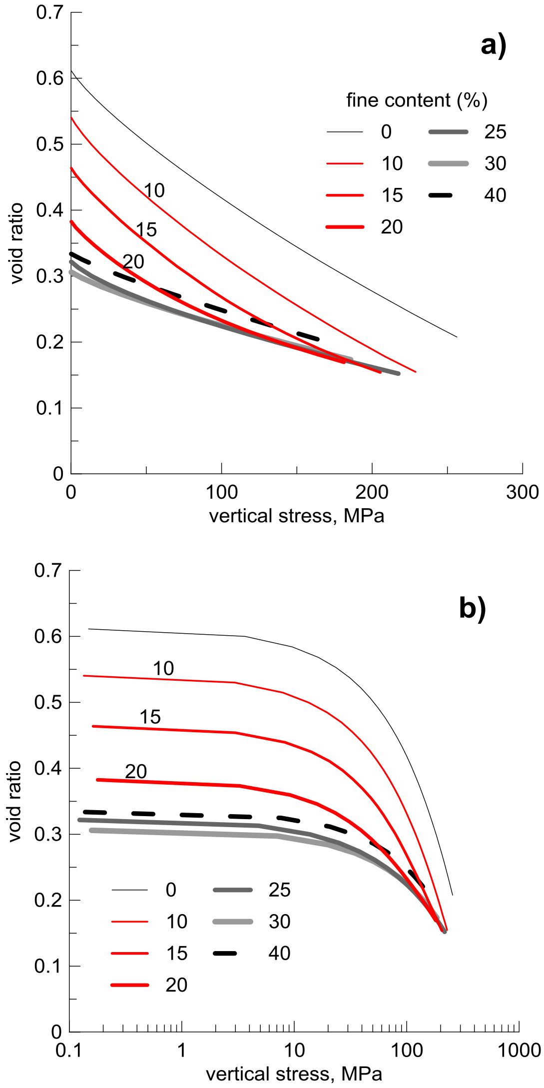

Figure 2. One dimensional compression curves for mixture samples plotted in a) a natural scale and b) a semi-log scale; the values in the legends indicate the percentage fines content . Color figure online.

The value of the threshold fines content using Rahman et al.'s approach is f_{thre} = 0.29, which agrees very well with the DEM results in Fig. 1 where f_{thre} = 0.30. The compression curves in term of the equivalent granular void ratio are shown in Fig. 4. Although the curves in Fig. 4 fall into a narrower band as compared to Fig. 3, the results are not necessarily better as there are still significant differences both in the initial void ratio and in the shape of the curves at high stress values. Carrera et al. (2011) applied the equivalent granular void ratio on a data set of 1D compression tests on a tailing material and did not obtain a unique normal compression line (NCL) but the NCL lines of different mixtures tended to intersect each other; this is also observed in Fig. 4. As concluded by Carrera et al. (2011), e^* has no physical meaning and at best can only be used as a qualitative estimation of the extent that the sand skeleton provides the major support for the applied force.

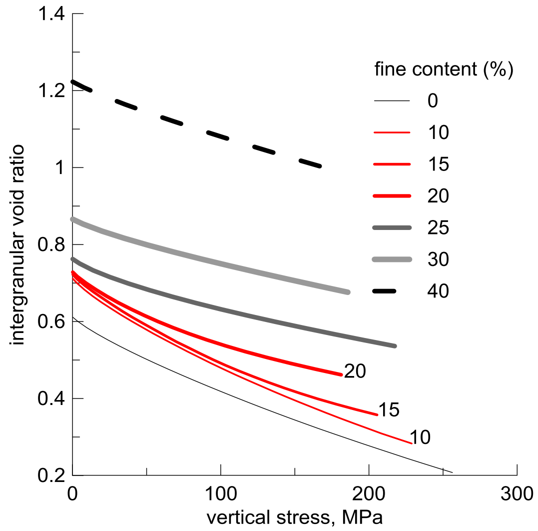

Figure 3. One dimensional compression curves in terms of the intergranular void ratio (b = 0). Color figure online.

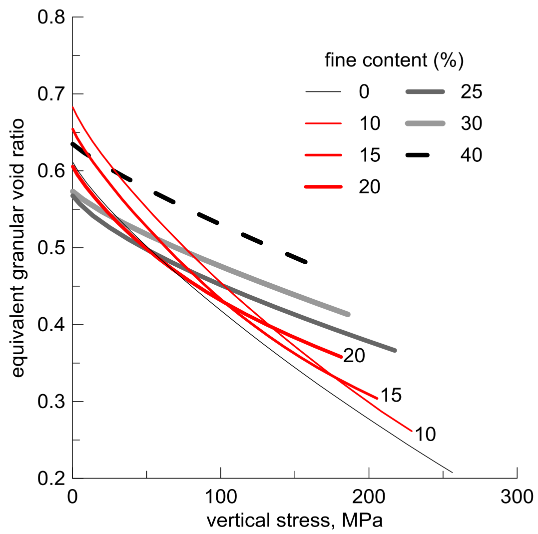

Figure 4. One dimensional compression curves in terms of the equivalent granular void ratio where b was calculated using the approach by Rahman et al. Color figure online.

2.2 *Identifying the meaning of active contacts*

Although the intergranular and equivalent granular void ratios were intended to be used as indices of the active contacts that sustain normal and shear forces, it is important to note that there is a high degree of force inhomogeneity for the force transmission through an assembly of discrete particles. The force transmission can be represented by two distinct classes called the strong force and the weak force contact networks (Radjai et al., 1998; Thornton & Antony, 1998). The strong forces were defined as contact forces contributing primarily to the macroscopic deviator stress and hence they determine the shear strength of the sample. The weak forces only contribute to the isotropic stress component or have a negligible contribution to the deviator stress. The force distinguishing between the strong forces and the weak forces is dependent on the PSD of the sample but it can be approximately taken as the average contact force in the system (Minh & Cheng, 2013b; Minh et al., 2014). For the calculation of e^*, it is not clear how to define a contact as an active contact. Two assumptions can be proposed: 1) an active contact is a force-transmitting contact, and 2) an active contact is a strong-force-transmitting contact. We calculated e^* using both assumptions and the results are presented in Figs. 5 to 9.

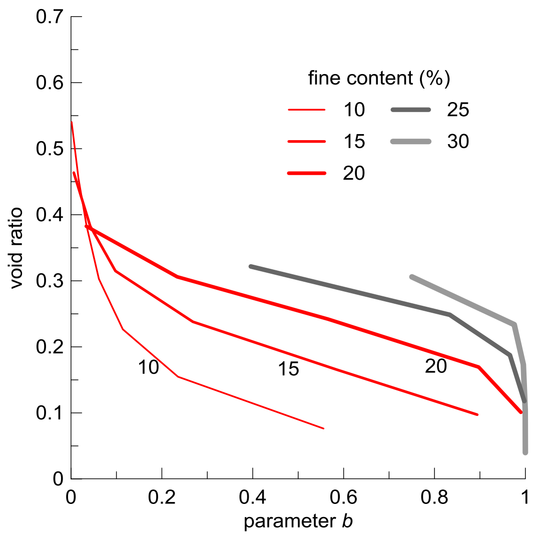

Figure 5. Variation of b-value for different fines content using DEM data where an active contact is defined as a force-transmitting contact. Color figure online.

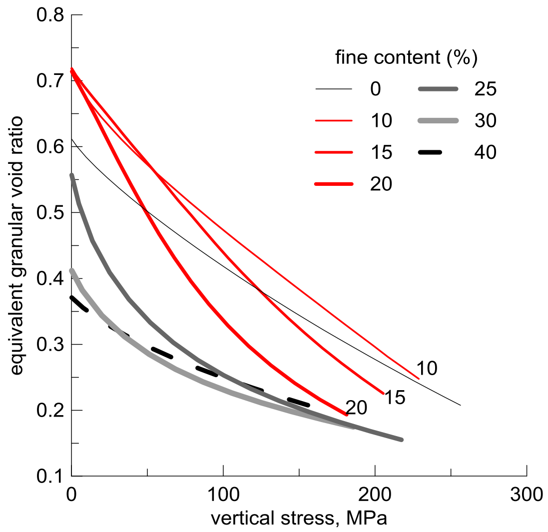

Figure 6. One dimensional compression curves in terms of the equivalent granular void ratio where b was calculated using DEM data for which an active contact is defined as a force-transmitting contact. Color figure online.

When a force-transmitting contact is considered an active contact, only fine particles that carry finite contact forces (excluding rattlers) are considered as the active fine particles. In the calculation of e^*, these active fine particles were counted into the solid volume whereas the inactive fine particles were counted as void. The b-value was calculated as the ratio between the volume of the active fine particles and the total volume of the fine particles. As the void volume decreases during compression, more fine particles become active in the force transmission and the value of b increases at smaller void ratio values as shown in Fig. 5. Knowing the value of the global void ratio e, using Fig. 5 we can determine the value of b during the compression process and finally e^* can be calculated from the values of e, b and f_c using Eq. 1. The values of e^* were calculated for the whole compression process and the results in term of e^* are shown in Fig. 6. Similar to Fig. 3, in Fig. 6 the curves of 10%-20% fines start from the same e^* value but then the curves start to deviate from each other. This means that this definition of active contacts is not valid. The resulting equivalent granular void ratios do not represent the active frictional contacts of the systems correctly; otherwise these samples should have similar behavior.

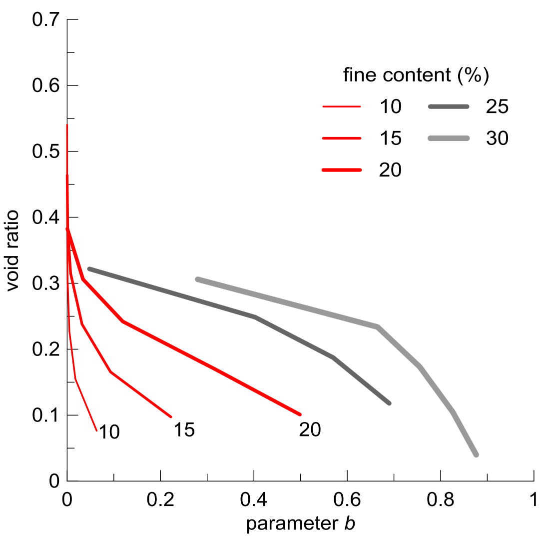

Figure 7. Variation of b-values for different fines content using DEM data where an active contact is defined as a strong-force-transmitting contact. Color figure online.

Calculation of the equivalent granular void ratio is repeated based on the second assumption that an active contact is a contact transmitting a strong force, the magnitude of which is greater than the average contact force in the system. These fine particles are called involved particles (Minh and Cheng, 2013b). Then, the fine particles are separated into two groups of the involved particles and the uninvolved particles where their volumes are counted differently toward the solid volume and the void volume. The variation of b-values is shown in Fig. 7. Compared to Fig. 5, the b-values are smaller when we adopt the second assumption of an active contact as there are fewer fine particles that are involved in the transmission of large forces in the system. The values of e^* were calculated from the values of e, b and f_c using Eq. 1 and the compression curves are shown in Fig. 8. The curves of the 10%-25% fines samples start from the same initial point in Fig. 8a; the 25% fines curve however deviates from the other curves afterwards whereas the 10%-20% fines follow the same path towards the end of compression. Figure 8b shows the results in a semi-log-scale plot and a unique normal compression line is only obtained for samples of 10%-20% fines contents. Fig.7 also shows that the parameter b is truly zero up to relatively high stresses and a relatively low void ratio (e.g. for the case with f_c = 10%, b = 0 when e > 0.22, this covers most of the stress range up to 170MPa. For the case with f_c = 15%, b = 0 when e > 0.32 and when the vertical stress < 80MPa, see Fig. 2); the start of the deviation from b = 0 however depends on fines content.

The fraction of active fine particles in the calculation of parameter b can now be defined as the fraction of the fine particles involved in the strong force transmission. Using microscopic analysis, the equivalent granular void ratio of a mixture can be explained as an index of the strong contacts that provide the primary source of shearing resistance in a granular system. This definition of the void ratio e^* has a physical meaning as it is linked to the shear-bearing-backbone comprised of the strong contacts in a granular system and the parameter b in the equation of e^* can be calculated explicitly as the fraction of the involved fine particles using the results from a DEM simulation. The strong contact force concept is a well-founded theory in the fields of particulate engineering and science.

In Figs. 8, the behaviour of the 30% and 40% fines samples are significantly different from the behaviour of samples having smaller fines contents and can be classified as another type of behaviour where both sand and fine particles are actively involved in the strong force transmission (Minh et al., 2014). For 0% fines, the behaviour is also not similar to that of the 10%-20% fines samples. If the 0% fines can only have sand-sand contacts, the 10%-20% fines samples can develop some sand-fine contact forces that have a small contribution to the deviator stress and this may explain the difference between the curves of 0% and 10%-20% fines in Fig. 8. In Minh et al. (2014), it was observed that for 20% fines some fine particles can be trapped between coarse particles and hence fine-sand contacts contribute to about 10% of the deviator stress but this is not reflected in the compression curves in Fig. 8. For the 25% fines sample, the fine-fine contacts start to contribute to the deviator stress and it is shown in Fig. 8 that the curve deviates from the 10%-20% fines curves at higher stress levels when this effect may become more significant. At the end of compression, about 70% (b = 0.7) of the fine particles are involved in the strong force transmission as shown in Fig. 7.

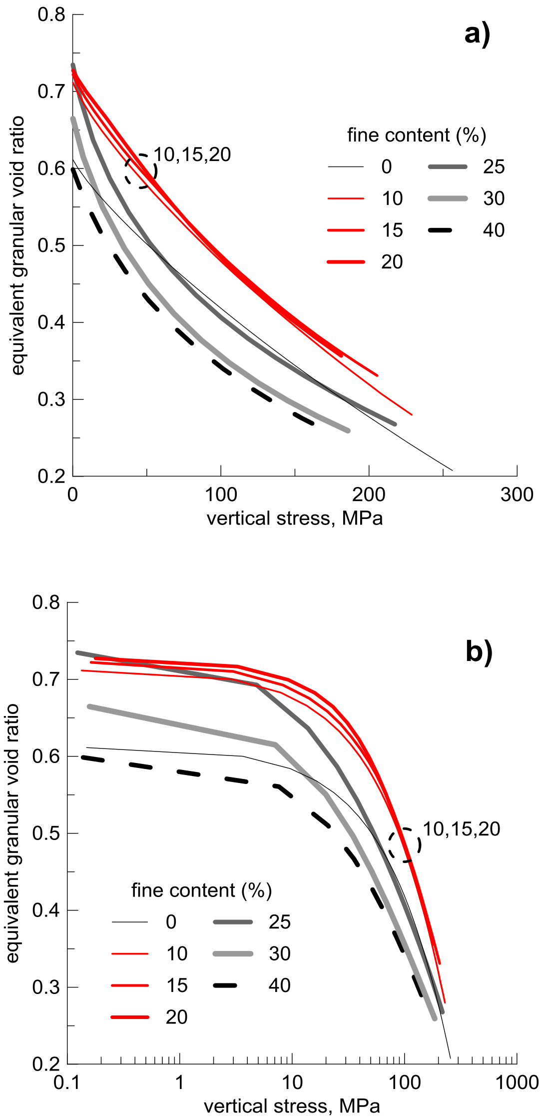

Figure 8. One dimensional compression curves in terms of the equivalent granular void ratio where *b* was calculated using DEM data in which an active contact is defined as a strong force-transmitting contact. Color figure online. a) natural-scale plot and b) semi-log-scale plot.

3 CONCLUSIONS

DEM simulations of the 1D compression of granular mixtures were conducted and the results were used to investigate the conceptual equivalent granular void ratio, which has been used quite commonly by soil mechanics experimentalists to address the liquefaction susceptibility of silty sand materials. The results showed that depending on the value of the fines content, a fraction of the fine particles can be involved in the strong force transmission in a granular system and the value of the parameter *b* can increase at smaller void ratios. For samples of fines content less than the threshold value, e^*, if correctly defined, can be used to obtain a unique normal compression line. The *b*-value is now calculated as the ratio between the volume of involved fine particles and the total volume of the fine particles. The application of e^* is however no longer valid when the fine-fine contacts start to contribute to the deviator stress; in this study this occurs at f_c = 25% instead of the threshold value f_c = 30% of the densest mixture.

Microscopic analysis provides a physical explanation for the equivalent granular void ratio where e^* can be considered as an index of the strong contacts that provides the primary source of shearing resistance in a granular system.

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