DEM analysis of the state parameter

Huang, X.^{a,b}, O'Sullivan, C.^a, Hanley, K. J.^a, Kwok, C.Y.^b

^a *Skempton Building, Department of Civil and Environmental Engineering, Imperial College London,
London SW7 2AZ, United Kingdom*

^b *Haking Wong Building, Department of Civil and Environmental Engineering, The University of
Hong Kong, Pokfulam Road, Hong Kong*

Abstract

Using a series of true-triaxial simulations, this study shows that the particulate Discrete Element Method (DEM) can capture the state-dependent drained and undrained response that is typical for sands. The most significant finding is that relationships between the initial state parameter and both the dilatancy at the peak strength and the difference between the peak and critical state strengths observed in the DEM simulations lie within the range defined by the experimental data. An exponential function is proposed to relate the difference between the peak and critical state strengths and the initial state parameter. As indicated by the DEM data, this relationship is independent of loading path (intermediate principal stress ratio). The correlations between the initial state parameter and both the peak strength and the stress ratio at the undrained instability state are qualitatively in accordance with previously published laboratory data. The DEM data agree well with the NorSand constitutive model. The relationships between the state parameter and both structural anisotropy at the peak stress as well as the coordination number are explored. These findings extend our current understanding of the capacity of DEM to capture the mechanical behaviour of granular materials and highlight the possibility of using DEM as a tool when developing advanced constitutive models.

Introduction

As is clearly articulated in Cundall (2001), the particulate implementation of the discrete element method (DEM) (Cundall & Strack, 1979) captures many of the unique mechanical characteristics of sands and other granular materials. The current study considers sand behavior within the critical state soil mechanics (CSSM) framework. Prior studies have demonstrated the ability of DEM to replicate critical-state type behaviour. For example, Thornton (2000) showed that when drained triaxial compression tests were simulated using DEM, a dense sample exhibited dilation while an equivalent loose sample contracted. Both samples had similar void ratios and stress states at large strain levels. More recently, a number of authors have confirmed that DEM simulations can give critical state loci in q - p' space and $e - \log(p')$ space (where p' is the mean effective stress, q is the deviator stress and e is the void ratio) (Ng, 2009; Yan & Dong, 2011; Zhao & Guo, 2013; Huang *et al.*, 2014). Here these earlier contributions are extended by considering the state parameter as proposed by Been and Jefferies (1985).

Been and Jefferies (1985) defined the state parameter (ψ) to be the difference between the current void ratio and the void ratio at critical state (e_{cs}) at the same p' . A positive value of ψ represents a loose state while a negative ψ value indicates a dense state. Triaxial test data show a convincing link between ψ and the mechanical response of soils, most notably, strength and dilatancy (e.g., Been & Jefferies 1985; Yang 2002). A number of recently-developed constitutive models for soil have explicitly considered ψ in their formulation, e.g., NorSand (Jefferies, 1993; Jefferies & Shuttle, 2002), Wood *et al.* (1994), Severn–Trent sand (Gajo & Wood, 1999) and the model proposed by Li and Dafalias (2000). Calibration of these models is complicated by the development of post-peak strain localizations in laboratory tests. There is also a scarcity of large-strain laboratory test data for 3D general loading conditions; this limits the ability to develop and to apply these models to field applications where the stress state is not axisymmetric. Prior studies simulating true-triaxial element tests (Thornton 2000; Ng 2004; Barreto & O'Sullivan 2012; Zhao & Guo 2013) have shown that DEM can replicate the failure envelopes proposed for real sands. Thus, if a DEM model can be shown

to capture the sensitivity of the material response to ψ that one would expect for a real sand, there is then potential to use DEM to advance critical state-based constitutive models for sand. This challenge is addressed here.

This paper shows that the DEM simulation data are in agreement with the empirically observed relationships between ψ and strength and between ψ and dilatancy, while extending prior understanding of the role of ψ by considering asymmetrical loading conditions. It is shown that the NorSand constitutive model (Jefferies, 1993; Jefferies & Shuttle, 2002) can be calibrated to capture the response observed in DEM. Finally, in an attempt to appreciate the fundamental basis of ψ , correlations between ψ and some particle-scale measures of response are presented.

Overview of DEM simulations

The DEM simulations presented here were performed using the open-source, MPI-parallelised LAMMPS code (Plimpton, 1995). Servo-control algorithms for periodically-bounded samples under drained (constant- σ'_3), constant-volume, constant- p' and constant intermediate stress ratio ($b = (\sigma'_2 - \sigma'_3)/(\sigma'_1 - \sigma'_3)$) conditions were implemented. The adapted code was validated against the analytical peak stress ratios proposed by Thornton (1979) for a face-centred cubic assembly of mono-sized rigid spherical particles.

102 simulations were performed using a virtual sand whose grading approximates that of Toyoura sand and are denoted as 'ST', while eight triaxial compression simulations ($b=0$) were carried out with samples having a grading similar to that of Dunkirk sand and are named as 'SD' as shown in Figure 1. For the ST grading the coefficient of uniformity and coefficient of curvature are $C_u = 1.386$ and $C_c = 0.983$; for the SD grading $C_u = 1.539$ and $C_c = 0.977$. The ST samples had 20,164 particles, while the SD samples contained 43,906 particles. A simplified Hertz-Mindlin (HM) contact model was used. The particle shear modulus (G) and Poisson's ratio (ν) were taken to be 29 GPa and 0.12 for the ST simulations and $G = 29.14$ GPa and $\nu = 0.2$ for the SD simulations. Gravity was not simulated.

All the particles were randomly generated within a cuboidal periodic cell and the samples were then isotropically compressed to target initial void ratios and stress states before shearing. True triaxial simulations were carried out under constant- b and constant- σ'_3 conditions using the ST samples. Eight different b values were investigated, i.e., $b = 0.0, 0.2, 0.3, 0.4, 0.5, 0.6, 0.8$ and 1.0 , varying from triaxial compression ($b=0.0$) to triaxial extension ($b=1.0$) conditions. A set of plane strain simulations (PS) were also conducted. Some additional constant-volume and constant- p' simulations were performed under triaxial compression and triaxial extension conditions. The constant-volume simulations approximate the undrained condition for fully-saturated sands. The interparticle friction coefficient (μ) during shearing for most of the simulations was 0.25 (i.e. unless otherwise specified, the simulations presented in the following text have $\mu = 0.25$). To investigate the effect of mineralogy $\mu = 0.1$ was applied to nine triaxial compression ST simulations and those samples are denoted as ST-b0.0- μ 0.1. Huang et al. (2014) have shown that it is not advisable to take $\mu \geq 0.5$ as this gives a critical state line in e - $\log(p')$ space that differs both qualitatively and quantitatively from that expected for a real sand.

State-dependent mechanical behaviour

Critical-state behaviour

Using the approach of Li & Wang (1998), e_{cs} is plotted against $(p'/p_a)^{0.7}$ ($p_a = 101.325$ kPa) in Figure 2 (a) giving a linear critical state line (CSL) for each set of simulations, i.e., $e_{cs} = \Gamma - \lambda \left(\frac{p'}{p_a}\right)^{0.7}$, where Γ is the intercept of CSL with $p'/p_a = 0$ axis and λ is the slope of the CSL. The confining pressures used for drained simulations in this study ranged from 50 kPa to 5 MPa; these give a very small variation in the critical-state void ratio ($e_{cs}=0.620\sim0.630$). In order to get a wider range of critical-state void ratios and thereby get a complete CSL, some constant-volume simulations were performed under both triaxial compression and triaxial extension loading conditions. The lowest void ratio simulated is around 0.578, which yielded a critical-state mean effective stress of 33.8 MPa for

the triaxial compression simulations and 40.7 MPa for the triaxial extension simulations. Constant p' simulations at corresponding stress levels were carried out to confirm that the constant-volume simulation results are valid. We restricted our stress levels to this limit to ensure that the maximum overlap ratio (i.e., the ratio between the interparticle overlap and the diameter of the smaller particle in the contact) was below 5% and thereby the basic small-overlap assumption of DEM was not violated. For the ST samples with $\mu = 0.25$, only the CSLs of the triaxial compression ($b = 0.0$) and triaxial extension ($b = 1.0$) tests are plotted for clarity and these CSLs bound the remaining true triaxial test data. Table 1 lists the values for the slope (λ) and intercept (I) of all the CSLs (note that the regression R-square values all exceeded 0.98). It is clear that while there is little variation in λ , I increases with increasing b . Wanatowski & Chu (2007) also observed that the position of CSL for plane strain in $e-p'$ space is above that for triaxial compression in their experiments on Changi sand. Note that in plane-strain conditions the b value is not a constant but evolves during shearing. In the simulations considered in the current study the b value reaches a constant value at the critical state.

Furthermore, the results presented by Wanatowski & Chu (2007) may be affected by the accuracy of their measurement of the intermediate stress, localization or the fact that they compared only triaxial compression and plane strain. In this numerical study, the stresses were accurately calculated, no localization was observed due to the use of periodic boundaries and a number of b values were studied in the DEM simulations. Therefore, our DEM data can be viewed as stronger evidence in support of the hypothesis that the position of the CSL in $e-p'$ space depends on b . This loading-mode dependency stems from the different micro structures induced by different loading modes (Huang, *et al.*, 2013). The CSLs for the ST simulations with $\mu = 0.1$ and for the SD simulations with $\mu = 0.25$ are both located below the CSLs of the ST simulations with $\mu = 0.25$. Figure 2 (b) illustrates the CSL in

terms of the deviatoric stress ($q = \sqrt{\frac{1}{2}((\sigma'_1 - \sigma'_2)^2 + (\sigma'_1 - \sigma'_3)^2 + (\sigma'_2 - \sigma'_3)^2)}$) and p' , where σ'_1 , σ'_2 , and σ'_3 are the major, intermediate, and minor principal effective stresses, respectively. The data in Figure 2 (b) and Table 1 indicate that the slope (M_{cs}) of the CSL in $q-p'$ space decreases consistently with increasing b . There is not a significant different between the M_{cs} values for the two relatively similar PSDs considered here. However, because the μ values used are < 0.5 , M_{cs} is

sensitive to μ , with M_{cs} decreasing from 0.6958 for $\mu = 0.25$ to 0.508 for $\mu = 0.1$ (Huang et al. 2014).

Although the M_{cs} value obtained in the current DEM simulations is much smaller than that of real Toyoura sand ($M_{cs} \approx 1.24$) (Cho et al., 2006), it is close to the M_{cs} value of glass beads ($M_{cs} \approx 0.82$) (Cavarretta, 2009).

Drained response

Figure 3 illustrates a state-dependent behaviour that is typical of sand by presenting the load-deformation response for three triaxial drained simulations each with a confining pressure (σ_3') of 500 kPa but different initial void ratios (e_0). The engineering definition of strains is used, i.e., the calculation of strains is based on the initial dimensions of the periodic cell. The initial state parameters (ψ_0) are -0.0414 for $e_0 = 0.588$, -0.0245 for $e_0 = 0.606$, and 0.0171 for $e_0 = 0.646$. As would be expected, the sample with the lowest ψ_0 ($e_0 = 0.588$) exhibited the highest peak strength (Figure 3 (a)) and dilated throughout shearing (Figure 3 (b)), while the sample with the highest ψ_0 ($e_0 = 0.646$) had the lowest peak strength, initially contracted prior to dilating and had an overall contractive response. It is worth noting that the behaviour of the DEM samples is very stiff which may explain the much smaller slope (λ) of the CSL in $e-(p'/p_a)^\alpha$ space than would be expected for real sand. The sample with a ψ_0 value of -0.0245 ($e_0 = 0.606$) had a response that was intermediate between these two scenarios. At large strain values (i.e., exceeding around 25%) all the samples had the same void ratio and stress ratio, indicative of an identical critical state which is independent of the initial packing density. Thornton (2000), Rothenburg & Krut (2004) and Guo & Zhao (2013) presented similar findings from their DEM simulations; however here the results are interpreted in terms of ψ_0 .

Undrained response

The stress-strain responses for three constant-volume simulations with $\sigma_3' = 5000$ kPa, and e_0 values of $\psi_0 = -0.0138$ ($e_0 = 0.604$), $\psi_0 = -0.0057$ ($e_0 = 0.612$), and $\psi_0 = 0.0019$ ($e_0 = 0.620$) are presented in Figure 4. Referring to Figure 4 (a), all the samples exhibited the typical three stages of loose to medium dense sand behaviour under undrained loading conditions as noted by Murthy et al. (2007),

i.e., an undrained instability state (IS), a phase transformation (PT) and a critical state (CS). It is also evident in Figure 4 (a) that q at the instability state, q at the phase transformation, and q at the critical state all decrease with increasing ψ_0 . Considering the stress paths in q - p' space in Figure 4 (b), it is clear that for all the samples, the mean effective stress initially decreases to the PT and increases thereafter until the critical states are attained. The maximum reduction in p' increases with increasing ψ_0 . Nevertheless, the critical state points of all the three simulations collapse to the same CSL passing through the origin; this is in line with the experimental observation of Wanatowski (2007). The instability lines, or flow liquefaction lines (FLL), which connect the origin and instability point in q - p' space (Lade, 1993) are also overlaid on Figure 4 (b). As shown in Figure 4 (b), the FLL is not unique but varies with ψ_0 . The slope of the FLL decreases with increasing ψ_0 , suggesting a reduction of liquefaction resistance with increasing ψ_0 . This agrees with Yang (2002).

Correlations between the state parameter and mechanical behaviour

Relationship between the state parameter and the strength

To quantitatively assess the similarity of the state-dependant response of DEM and sand reported by Been and Jefferies (1985), the peak angle of shearing resistance (ϕ'_p) for drained simulations under both constant σ'_3 and constant p' conditions is plotted against the initial state parameter (ψ_0) in Figure 5. The experimental data **from triaxial compression tests** for real sands documented in Jefferies & Been (2006) are also included in Figure 5. It is clear that the general trend in both cases is a decrease of ϕ'_p with increasing ψ_0 . The ϕ'_p values for the DEM simulations are consistently below the experimental ϕ'_p values; this can be attributed to the use of spherical particles which cannot capture the interlocking effects observed in irregular real sand particles. Many prior studies have shown either experimentally (e.g., Cho et al. (2006)) or using DEM (e.g., Maeda et al. 2009) that the strength depends on particle geometry, and so it is not surprising that the DEM data, obtained using spherical particles, lie below the experimental data that were obtained using real, non-spherical grains. The initial isotropic fabric in the DEM simulations may also contribute to the difference between the experimental and DEM data. For the DEM simulations with $\mu = 0.25$, the cases with intermediate

principal stress ratios of $b = 0.0$ and $b = 0.5$ give lower and upper bounds respectively to the ϕ'_p values. This is in accordance with the variation of peak strength with intermediate stress ratio noted by Ng (2004) and Huang et al. (2013) amongst others and captured in 3D failure criteria (e.g., Lade & Duncan (1975)). The DEM simulations with $\mu = 0.1$ give ϕ'_p values that are lower than those observed for $\mu = 0.25$; the dependency of this relationship on the interparticle friction may indicate a dependency on mineralogy in physical tests. The trend is observed for both DEM sample types - SD triaxial simulations give responses that are close to those observed for the ST simulations with $b = 0.0$.

Taylor (1948) proposed that soil strength can be decomposed into a dilational component and an intrinsic component, leading to development of the stress-dilatancy theory (Rowe, 1962). Following the approach of Been and Jefferies (1985), the dilational component of the strength at peak for the DEM simulations, i.e., $\phi'_p - \phi'_{cs}$, is plotted against ψ_0 in Figure 6. The experimental data reported by Jefferies and Been (2006) are also included in Figure 6. It is clear that the responses observed in the DEM simulations lie within the bounds of the reported experimental data. This indicates that the relationship between $\phi'_p - \phi'_{cs}$ and ψ_0 is not shape-dependant; the DEM parametric study also reveals a lack of dependence upon b and perhaps μ as well. The $\phi'_p - \phi'_{cs}$ values of the SD samples under triaxial compression conditions ($b=0.0$) are slightly higher than those of the ST samples under the same loading conditions which may be due to the small difference in grading. The experimental data exhibit more scatter around the general trend than the DEM data. This may be attributable to the differences in initial fabric due to the use of different sample preparation methods. All the DEM samples start from an isotropic state, so any fabric dependency will not be evident from the simulation results. Figure 6 complements the idea of Bolton (1986) that the dilational contribution to the overall strength depends on both initial packing density and stress state. Figure 6 also indicates that the dependency of the dilational contribution to the overall strength on the initial states is independent of b .

Yang (2002) proposed an exponential correlation between the stress ratio at instability state ($\eta_{IS} = q_{IS}/p'_{IS}$) and ψ_0 to illustrate the state-dependent undrained strength of sands:

$$\eta_{IS} = \frac{M}{B} e^{A\psi_0} \quad (1)$$

where M is the critical-state stress ratio and A and B are fitting parameters. For the DEM for undrained triaxial compression simulations listed in Table 2 (i.e., $b=0$), $A \approx -19.77$ and $B \approx 1.72$ with $M = 0.695$; the best-fit line and data are illustrated in Figure 7 .

Relationship between the state parameter and dilatancy

Bolton (1986) clearly links the difference between the mobilized angle of shearing resistance and ϕ'_{cs} to dilatancy and Been and Jefferies (1985) proposed that the dilation rate ($D^p = -d\varepsilon_v^p / d\varepsilon_q^p$) at the peak stress ratio (D^p_{max}) is linked to ψ_0 . Figure 8 plots D^p_{max} against ψ_0 for the DEM dataset and also includes the experimental data presented in Jefferies and Been (2006). Note that D^p was calculated using total strains, rather than the plastic strain components assuming that the elastic strain components are negligible at this point. The work conjugate shear strain (ε_q) proposed by Jefferies & Shuttle (2002) is used to ensure that the work done by the stress invariants (q and p') equals that calculated considering the principal stresses and strains.

$$\varepsilon_q = \frac{s_1\varepsilon_1 + s_2\varepsilon_2 + s_3\varepsilon_3}{q} \quad (2)$$

where $s_1 = (2\sigma'_1 - \sigma'_2 - \sigma'_3)/3$, $s_2 = (2\sigma'_2 - \sigma'_3 - \sigma'_1)/3$ and $s_3 = (2\sigma'_3 - \sigma'_1 - \sigma'_2)/3$. Equation 2 reduces to the traditional definition of deviatoric strain, i.e., $\varepsilon_q = \frac{2}{3}(\varepsilon_1 - \varepsilon_3)$, under triaxial conditions. Just as was the case when $\phi'_p - \phi'_{cs}$ was plotted against ψ_0 , plotting D^p_{max} against ψ_0 for the DEM data indicates a unique relationship that does not depend on b and the DEM data lie within the range defined by the experimental data.

It is also interesting to consider the state parameter when the peak stress is mobilized, ψ_p , i.e. the difference between the void ratio at the peak and e_{cs} at the same p' value. Following Jefferies & Shuttle (2002), D^p_{max} and ψ_p can be represented by following relationship considering $D^p_{max} = 0$ at critical state ($\psi_p = 0$):

$$D_{max}^p = -\chi \cdot \psi_p \quad (3)$$

As shown in Figure 9 (a), this linear correlation is also evident for the DEM simulations. Figure 9 (b) shows that χ varies systematically with b and μ for the ST samples. The DEM simulation results for the two PSDs considered do not noticeably differ ($\chi_{tc} = 6.108$ for the ST samples and $\chi_{tc} = 6.467$ for the SD samples) which is attributable to the similarity in grading.

Strength and dilatancy

Figures 10 (a) and (b) plot the peak strength against the dilatancy at peak (D_{max}^p) of DEM data in terms of angle of shearing resistance (ϕ'_p) and stress ratio (η_p), respectively. The resultant linear correlation between ϕ'_p and D^p corresponds with what we would expect for a real sand (e.g., Vaid & Sasitharan (1991)). Considering the ST simulations with $\mu = 0.25$, the slope and position of the best-fit lines appear to be dependent on b , in line with the dependency of strength on b as observed by Ng (2004) and Huang et al. (2013). The best-fit lines for the ST simulations with $\mu = 0.1$ are located below those for $\mu = 0.25$. The SD DEM data collapse to give effectively the same trend that was observed for the ST data with $\mu = 0.25$ and $b = 0.0$, which again may be due to the similarity in grading of these two materials.

According to stress-dilatancy theory, the critical state strength can be estimated from the strength - dilatancy relationship shown in Figure 10 by considering the critical state as $D^p = 0$, i.e., the intercept of the linear best-fit function. Building on the idea proposed by Bishop (1971), Vaid and Sasitharan (1991) suggested this might be a valid method to estimate the critical-state strength from the peak strength, noting that it is not always easy to achieve the large strains associated with the critical state. Figure 11 (a) and (b) support this idea as the critical-state strengths predicted in this way are in good agreement with the measured critical-state strengths. The small difference between the measured and predicted values may be attributable to the use of total strains instead of plastic strains when calculating the dilatancy.

NorSand calibration

A number of constitutive models for sands have been proposed based on critical state soil mechanics (CSSM) and explicitly consider the state parameter (e.g., Jefferies 1993; Manzari & Dafalias 1997; Gajo & Wood 1999; Li & Dafalias 2000). Development and calibration of these models is hindered by the lack of available data on critical state behaviour under 3D generalised stress states. The data presented include a number of non-axisymmetric stress simulations and to illustrate the potential for such a dataset to aid in the development of constitutive models, the NorSand model (Jefferies, 1993; Jefferies & Shuttle, 2002) is calibrated against this dataset.

Overview of NorSand

The NorSand model was presented in Jefferies (1993) and Jefferies & Shuttle (2002). Perhaps the most detailed description of NorSand can be found in Jefferies & Been (2006). NorSand is essentially an isotropic elasto-plastic model and thus is suited to modelling the DEM simulations presented here which start from isotropic states. The implementation of 3D NorSand in this study follows Jefferies & Shuttle (2002). Modifications to the original NorSand modelling software downloaded from the website of the geotechnical group of the University of British Columbia (Jefferies & Shuttle (2005)) include:

- (a) The substitution of the CSL expression in terms of e and $\log(p')$ with the power-law relationship proposed by Li & Wang (1998).
- (b) The complete formulation of NorSand as introduced in Jefferies & Been (2006) was implemented.
- (c) The state parameter at image state rather than the current state was used to calculate M_i , dp'/p'_i and $(dp'/p'_i)_{max}$, where p'_i is the mean effective stress at image state at which $D^p = 0$ but $\dot{D}^p \neq 0$.
- (d) The interpolated variation of the critical-state stress ratio with Lode angle θ ($\sin(3\theta) = -13.5s_1s_2s_3/q^3$) used is that proposed by Jefferies & Shuttle (2011) as it agrees well with the DEM data as shown in Figure 12.

$$M_{\theta} = M_{tc} - \frac{M_{tc}^2}{3+M_{tc}} \cos\left(\frac{3\theta}{2} + \frac{\pi}{4}\right) \quad (4)$$

(e) 3D NorSand was implemented for true triaxial tests under constant- b and constant- σ'_3 conditions.

Calibration of NorSand

NorSand uses the critical-state parameters Γ , λ and M_{cs} . The plasticity parameters considered are H , the hardening modulus, χ , which reflects the variation of D^p_{max} with ψ_p , and N which describes the strength and dilatancy relationship. The elastic parameters are the elastic rigidity, $I_r = G/p'$, and the Poisson's ratio, ν . Many of the NorSand model parameters can be determined from the data presented above: Γ , λ and M_{cs} are listed in Table 1 (note that the power-law interpretation of the CSL is adopted), χ can be determined from Figure 9 (b), N equals to $1 - k$, where k are the slopes of the linear relationships shown in Figure 10 (b), and a Poisson's ratio of 0.2 is reasonable as ν does not vary greatly between different types of granular materials. The input initial shear modulus (G) for the current DEM dataset was determined from the elastic range of the q - ε_q curve using small strain probes (Zheng, 2014) and can be expressed as:

$$G = \frac{139967.7042 \times (1.1666 - e)^2}{1 + e} (p')^{0.36554} \quad (5)$$

The G values determined by Equation 5 are several times larger than the G values of real Toyoura sand due to the stiffer response of the DEM samples. The corresponding I_r values can be determined, thereby leaving H as the only parameter to calibrate. Calibration of H was achieved by minimising the squared deviations between the DEM data for deviatoric stress (q) versus axial strain (ε_a) and the corresponding NorSand response considering the full axial strain range.

Performance of NorSand under 3D general loading conditions

Figures 13 and 14 compare the stress-strain behaviour modelled using NorSand with the measured stress-strain behaviour in DEM simulations for a dense sample ($e_0 = 0.549$, $\sigma'_3 = 300$ kPa, $\psi_0 = -0.0823$) and a loose sample ($e_0 = 0.646$, $\sigma'_3 = 500$ kPa, $\psi_0 = 0.0171$) respectively. For clarity, only data for

simulations of triaxial compression ($b = 0.0$), plane strain (PS) and true triaxial compression with $b = 0.8$ are presented. The H and I_r values vary with the initial state but are found to be independent of the intermediate stress ratio as listed in Table 3.

Referring to Figure 13 (a), the deviatoric stress of the dense sample initially increases sharply to the peak followed by an obvious softening response and becomes constant at critical state. Although the modelled behaviour slightly over-estimates the peak strength of the DEM simulation results for all the stress conditions considered, there is in general a good agreement with the DEM data. As illustrated in Figure 13 (b), in the small strain regime, the measured and modelled volumetric behaviour is closely matched, showing an initially contractive followed by a dilative response. However, the modelled results deviate from the DEM simulation data as the strain levels increase. This is most likely a consequence of neglecting the high-order products of the infinitesimal strain increments in the calculation of the volumetric strain increment as the engineering definition of strain is adopted in the current study. These high-order products become increasingly significant as the strain level increases. The difference between the model results and the DEM data decreases when the critical state is approached due to the constraints imposed by the same CSL existing in both q - p' and e - $\log(p')$ spaces for both the NorSand modelling results and the DEM simulations. Similar observations can be made for the loose sample, as illustrated in Figure 14.

Similarly, effective calibration was achieved for the other DEM simulations. The large number of simulations allowed the factors which determine the modelling hardening modulus (H) to be established. Referring to Figure 15, the linear relationship between H and ψ_0 proposed by Jefferies & Been (2006) considering experimental data is also evident considering the calibration against the DEM data. The slope of the H - ψ_0 relationship for the DEM data is higher than for the experimental data for real sand considered by Jefferies & Been (2006). A number of factors may be responsible for the difference between the H values for real sand and the H values obtained in the DEM simulations, including the influence of particle shape, mineralogy, grading and initial fabric. Furthermore, the higher H values obtained in DEM simulations can also possibly be attributed to the lower location of

the CSL in e -log (p') space of the DEM data in comparison to the experimental data. Given the same ψ_0 , the void ratio of DEM data is actually much smaller than the experimental data, which may result in a stiffer response. This void ratio difference also explains the higher H value for the SD simulations in comparison with the ST simulations.

State parameter and particle-scale measures

DEM allows the link between the state-dependent material behaviour and the internal topology, or fabric, of the material to be established. The coordination number, Z , is a measure of the packing density of a granular assembly and is defined as $Z = 2N_c/N_p$, where N_c and N_p are the number of contacts and the number of particles, respectively. Huang *et al.* (2013) showed that the critical states for the true triaxial tests presented here can be described by a relationship in Z -log (p') space that is independent of the intermediate stress ratio and loading conditions, indicating that Z is a micro-scale measure of 'state'. A micro-scale state parameter ($Z-Z_{cs}$) is proposed here to be the difference between the current Z value and the value of Z at the critical state corresponding to the same p' , similar to the definition of traditional state parameter. Z_0 is the initial coordination number, and Figure 16 (a) shows that there is a correlation between Z_0-Z_{cs} and D_{max}^p that appears to be independent of loading path, and data of ST-b0.0- μ 0.1 and SD-b0.0 tend to align in the same trend as that of ST- μ 0.25, in line with the relationship between ψ_0 and D_{max}^p . There is also a good correlation between Z_0-Z_{cs} and peak strength. While Barreto & O'Sullivan (2012) and Huang, *et al.* (2014) both observed that there is no simple functional relationship between either Z and e or Z and p' during shearing, Figure 16 (b) reveals a clear linear correlation between Z_0-Z_{cs} and ψ_0 for drained simulations, which may possibly account for the good correlations between Z_0-Z_{cs} and both strength and dilatancy. Considering that the same isotropic compression method was used and particles were spherical, whether these observations are also applicable to samples generated by other methods which may possibly yield an initially preferential fabric direction and thereby a different Z_0 (e.g, Ng, 2004a) requires further exploration.

While the material considered here is initially isotropic, the stress conditions during shearing will induce an anisotropic fabric and the structural anisotropy can be quantified by the fabric tensor (Satake, 1982),

$$\Phi_{ij} = \frac{1}{N_c} \sum_{k=1}^{N_c} n_i^k n_j^k \quad (6)$$

where n_i^k denotes the unit contact normal. Here a deviatoric fabric is considered, whose definition resembles the definition of the deviatoric stress: $\Phi_d = \sqrt{\frac{1}{2}((\Phi_1 - \Phi_2)^2 + (\Phi_1 - \Phi_3)^2 + (\Phi_2 - \Phi_3)^2)}$, where Φ_1 , Φ_2 and Φ_3 are the major, intermediate, and minor principal fabrics respectively. As shown in Figure 17, when Φ_d is calculated considering all the contacts, Φ_d at the point where peak strength is mobilized decreases with increasing ψ_0 . The data for the simulations using $\mu = 0.1$ are generally located below the data for simulations with $\mu = 0.25$. For simulations using $\mu = 0.25$, the relationship between Φ_d and ψ_0 for different loading paths tends to converge for $\psi_0 \leq -0.1$, more scatter is evident for $\psi_0 > -0.1$. In their DEM simulations, Sazzad & Suzuki (2013) noted a linear relationship between the stress ratio (q/p') and a strong deviatoric fabric Φ_d^s which is calculated by considering only strong contacts (i.e., contacts transmitting above-mean contact forces). Figure 18 (a) shows the variation of Φ_d^s at peak strength ($\Phi_{d,peak}^s$) with ψ_0 . It is evident that the locations of $(\Phi_{d,peak}^s, \psi_0)$ drift systematically downwards with increasing b . The value of $\Phi_{d,peak}^s$ for $\mu = 0.1$ is smaller than that for $\mu = 0.25$ at the same b . This agrees with the variation of critical stress ratio with b and μ as listed in Table 1. Just as in the case of the relationship between $\phi'_p - \phi'_{cs}$ and ψ_0 , when the structural anisotropy at critical state is removed from the anisotropy at peak strength, the difference between the different loading paths and different μ cases becomes less noticeable as illustrated in Figure 18 (b). The strong contacts transmit most of the forces so there is a strong link between Φ_{ij}^s and σ_{ij} . Therefore the correlations with Φ_d^s presented in Figure 18 may arise from the existence of the correlations with ϕ' presented in Figures 5 and 6.

Conclusions

This study has explored the state-dependent mechanical behaviour of granular materials using DEM simulations of true triaxial tests. A particular emphasis is placed on examining the link between the state parameter and the mechanical behaviour that had previously been established by Jefferies and Been (Been & Jefferies, 1985; Jefferies & Been, 2006). The main findings can be summarized as follows:

It has been shown that the DEM simulations can capture the relationships between the state parameter and both soil strength and dilatancy observed in laboratory tests reported by Jefferies and Been (2006). In particular, the relationships between the state parameter, ψ_0 , and both the dilational component of strength ($\phi'_p - \phi'_{cs}$) and the dilatancy at peak (D^p_{max}) obtained in the DEM simulations quantitatively agree with the empirical data presented by Jefferies and Been (2006). These relationships were shown to be unique and independent of the loading path. In drained triaxial loading conditions, the peak strength (ϕ'_p) was observed to decrease systematically with increasing initial state parameter (ψ_0), giving a trend that is qualitatively in agreement with the empirical data reported in Jefferies and Been (2006). The DEM data also showed that this relationship depends on the intermediate stress ratio. For DEM simulations of constant-volume triaxial tests, the strength was observed to systematically increase with decreasing ψ_0 , in line with Yang (2002). Thus, these qualitative agreements also strengthen the case for the ability of DEM to capture the type of response we would expect within the critical state soil mechanics framework.

NorSand (Jefferies, 1993; Jefferies and Shuttle, 2002), an isotropic critical state-based constitutive model originated from the laboratory-testing data, was shown to be able to effectively model the DEM data, following the same calibration approach one would apply to an experimental dataset. The good agreement between the DEM simulation data and the NorSand modelling results indicates the potential for DEM to be used in the development of continuum constitutive models.

Good correlations were observed between the micro-scale state parameter ($Z_0 - Z_{cs}$) and both strength and dilatancy. This can be attributed to the linear relationship between $Z_0 - Z_{cs}$ and ψ_0 . DEM simulations generate the data necessary to quantitatively link the granular material fabric to the overall mechanical response. Here, the deviatoric fabric for the strong contacts, i.e., the above-mean contacts, was seen to agree with the variation of the macro-strength with ψ_0 . This is perhaps unsurprising as the strong contacts are known to play a dominant role in stress transmission; however, no such correlation can be observed when considering the structural anisotropy of all contacts.

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Notation

b Intermediate stress ratio $b = (\sigma'_2 - \sigma'_3)/(\sigma'_1 - \sigma'_3)$

D^p Dilatancy $D^p = d\varepsilon_v^p/d\varepsilon_q^p$

e Void ratio

H Hardening modulus of the NorSand model

I_r Elastic rigidity of the NorSand model

M_{cs} Stress ratio at the critical state

M_i Stress ratio at the image state

N Volumetric coupling parameter in stress dilatancy of the NorSand model

p' Mean effective stress $p' = (\sigma'_1 + \sigma'_2 + \sigma'_3)/3$

q Deviatoric stress $q = \sqrt{\frac{1}{2}((\sigma'_1 - \sigma'_2)^2 + (\sigma'_1 - \sigma'_3)^2 + (\sigma'_2 - \sigma'_3)^2)}$

$s_{1,2,3}$ $s_1 = (2\sigma'_1 - \sigma'_2 - \sigma'_3)/3$, $s_2 = (2\sigma'_2 - \sigma'_3 - \sigma'_1)/3$ and $s_3 = (2\sigma'_3 - \sigma'_1 - \sigma'_2)/3$

Z Coordination number

χ Dilatancy parameter of the NorSand model

ε_v Volumetric strain $\varepsilon_v = \frac{\varepsilon_1 + \varepsilon_2 + \varepsilon_3}{3}$

ε_q Deviatoric strain $\varepsilon_q = \frac{s_1\varepsilon_1 + s_2\varepsilon_2 + s_3\varepsilon_3}{q}$

η Stress ratio q/p'

ϕ' Angle of shearing resistance ($^\circ$)

Φ_{ij} Fabric tensor (See Equation 6)

Φ_d Deviatoric fabric $\Phi_d = \sqrt{\frac{1}{2}((\Phi_1 - \Phi_2)^2 + (\Phi_1 - \Phi_3)^2 + (\Phi_2 - \Phi_3)^2)}$

μ Interparticle friction coefficient

ψ State parameter

λ Slope of the critical state line in the $e-(p'/p_a)^\alpha$ space

σ'_1 Major effective principal stress

σ'_2 Intermediate effective principal stress

σ'_3 Minor effective principal stress

Γ Intercept of the critical state line in the $e-(p'/p_a)^\alpha$ space with the axis $p' = 0$

θ Lode angle $\sin (3\theta) = -13.5s_1s_2s_3/q^3$

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Table 1 Summary of the critical state parameters

	0.0	0.2	0.3	Plane strain	0.4	0.5	0.6	0.8	1.0	$\mu =$ 0.1	Dunkirk
M_{cs}	0.695	0.673	0.647	0.634	0.627	0.609	0.594	0.575	0.573	0.508	0.702
Φ'_{cs} (°)	18.2	19.8	20.2	20.8	20.5	20.5	20.3	19.5	18.5	13.5	18.3
λ	0.000923	0.000761	0.000883	0.000753	0.000836	0.0009	0.000831	0.000841	0.00096	0.0011	0.000789
Γ	0.632	0.633	0.634	0.635	0.635	0.637	0.639	0.640	0.641	0.592	0.584

Table 2 Initial state parameter (ψ_0) and stress ratio at instability state (η_{IS}) for undrained simulations

ID	e_0	$\sigma_3'^0$	ψ_0	η_{IS}
0.613-500	0.613	500	-0.0162	0.528
0.6163-500	0.6163	500	-0.0129	0.502
0.619-500	0.619	500	-0.0102	0.474
0.6165-1000	0.6165	1000	-0.0109	0.495
0.6166-2000	0.6166	2000	-0.008	0.466
0.6165-5000	0.6165	5000	-0.0014	0.424
0.604-5000	0.604	5000	-0.0138	0.540
0.6122-5000	0.6122	5000	-0.0057	0.475
0.6198-5000	0.6198	5000	0.0019	0.403
0.6245-5000	0.6245	5000	0.0066	0.338

Table 3 Input modelling parameters for NorSand

	Plasticity									Elasticity					
	H			χ			N			I_r			ν		
	b = 0.0	PS	b = 0.8	b = 0.0	PS	b = 0.8	b = 0.0	PS	b = 0.8	b = 0.0	PS	b = 0.8	b = 0.0	PS	b = 0.8
$e_0 =$ 0.549, $\sigma'_3 =$ 300 kPa	281	281	281	6.108	5.9556	5.0411	0.4982	0.582	0.5134	924.18	924.18	924.18	0.2	0.2	0.2
$e_0 =$ 0.646, $\sigma'_3 =$ 500 kPa	41	41	41	6.108	5.9556	5.0411	0.4982	0.582	0.5134	446.91	446.91	446.91	0.2	0.2	0.2

Figure1 Comparison between grading curves of numerical samples and the experimental grading

(a) CSL in $e-(p'/p_a)^{0.7}$ space

(b) CSL in $q-p'$ space

Figure 2 Critical-state behaviour

(a) Stress ratio

(b) Void ratio

Figure 3 Triaxial drained simulations under the same confining pressure ($\sigma'_3=500\text{kPa}$)

(a) Variation of q with axial strain

(b) Stress paths

Figure 4 Constant-volume simulations under the same confining pressure ($\sigma'_3=5000\text{kPa}$)

Figure 5 Initial state parameter (ψ_0) and peak angle of shearing resistance (ϕ_p), DEM simulation results presented along with the experimental data from triaxial compression tests reported in Jefferies and Been (2006)

1
2 Figure 6 Initial state parameter (ψ_0) and stress dilatancy angle of shearing resistance ($\phi_p - \phi_{cs}$), DEM
3 simulation results presented along with the experimental data from triaxial compression tests reported
4 in Jefferies and Been (2006)

1

2

3 Figure 7 Relationship between the stress ratio at instability state (η_{IS}) and initial state parameter (ψ_0)4 for undrained triaxial compression simulations ($b=0$)

5

Figure 8 Relationship between the peak dilatancy (D^p_{max}) and the initial state parameter (ψ_0), DEM simulation results presented along with the experimental data from triaxial compression tests reported in Jefferies and Been (2006)

Figure 9 Relationship between the dilatancy at peak (D^p_{max}) and the state parameter at peak (ψ_p)

(a) Dilatancy at peak against peak angle of shearing resistance

(b) Dilatancy at peak against peak stress ratio

Figure 10 Relationship between the peak strength and dilatancy at peak

Figure 11 Comparison between the measured critical state strength and the critical state strength predicted from the strength- dilatancy relationship

Figure 12 Variation of critical state stress ratio (M_{cs}) with Lode angle (θ)

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2
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Figure 13 Comparison between the NorSand modelling results and the DEM data for a dense sample ($e_0 = 0.549$, $\sigma'_3 = 300$ kPa, $\psi_0 = -0.0823$) (The solid lines represent $b=0.0$, the dashed lines correspond to PS and the dot lines indicate $b=0.8$. The DEM data are in black, while the NorSand modelling curves are in grey.)

(a) Stress ratio

(b) Volumetric strain

Figure 14 Comparison between the NorSand modelling results and the DEM data for a loose sample ($e_0 = 0.646$, $\sigma'_3 = 500$ kPa, $\psi_0 = 0.0171$) (The solid lines represent $b=0.0$, the dashed lines correspond to PS and the dot lines indicate $b=0.8$. The DEM data are in black, while the NorSand modelling curves are in grey.)

1
2

3
4

Figure 15 Variation of hardening modulus (H) with initial state parameter (ψ_0)

(a) $Z_0 - Z_{cs}$ and D_{max}^p

(b) $Z_0 - Z_{cs}$ and ψ_0

Figure 16 Relationships between micro-scale state measurement and macro-scale state measurement

Figure 17 Relationship between the deviatoric fabric at peak and initial state parameter

Figure 18 Correlations between the strong deviatoric fabric and initial state parameter