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Micromechanics-based assessment of reliability and applicability of boundary measurements in symmetrical direct shear test

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ABSTRACT

The development of discrete element method (DEM) provides an efficient tool to examine and appraise the performance of direct shear apparatus (DSA) to overcome the ambiguities arise from the complexity of stress and strain distributions involved. This paper presents DEM analyses of both macro and micromechanics responses of three-dimensional (3D) dense samples of 102248 glass spheres tested in virtual symmetrical DSA using the computer code SiGran. Particular emphasis is placed on the validation of the DEM model by comparing the results of DEM simulations with their physical counterparts at the macro-scale. The performance of the physical direct shear apparatus is optimized by exploring modifications to the symmetrical test configuration. The numerical results provide quantitative data on different forms of energy consumed during shearing confirming other published physical and numerical results found in the literature. The virtual DSA results are also discussed in terms of the coaxiality between the principal stresses and the principal strains increments directions as well as the deviation of the zero extension direction from the horizontal direction. The micro-scale results showed that peak state parameters obtained from the symmetrical arrangement, adopted in this study, are very close to those of an ideal simple shear test, as it permits a uniform deformation within the developed shear band, a horizontal orientation of the zero linear extension, and a coaxiality of principal stresses and incremental strains at the peak state. In other words, the micro-scale results, presented in this study, provide new evidence that corroborates the further use of the boundary measurements in physical symmetrical direct shear tests.

Keywords: Laboratory tests, Numerical analysis, discrete element method, boundary measurements

Introduction

Knowledge of the main factors dominating the strength characteristics of geomaterials has attracted the attention of many researchers and geotechnical engineers since the early 1920s and the relevant literature is abundant (Terzaghi 1970; Bolton 1986). The core of these researches relied primarily on laboratory experimentations on drained or undrained soil samples in standard geotechnical apparatuses that were developed during this period. Through this long history of research, a common understanding has been gradually formed among the geotechnical community on the inter-particle friction angle, particle rearrangement, and dilation. In the recent decades, the research effort has been more directed towards understanding the fundamental micro-mechanism underlying the strength response and deformation properties of soil as it is, in fact, essential to better interpret important geotechnical phenomena such as sand boils and soil liquefaction (Seed and Lee 1966; Ishihara 1993).

Today's understanding of the micro-scale response of soil is chiefly based on numerical simulations of traditional soil tests, such as triaxial and direct shear tests. The direct shear apparatus (DSA) is, in particular, one of the oldest and most commonly used laboratory devices, and was constructed by Collin as early as 1846 for slope stability analysis (Skempton 1949). Developing the DSA in its present form dates back to Krey (1926), which later modified by Casagrande (1936) and Terzaghi and Peck (1948) to account for the vertical expansion and contraction measurements. However, since the exact state of stress within the shear band was unknown, the reliability of traditional direct shear interpretation was questionable (Morgenstern and Tchalenko 1967; Saada and Townsend 1981).

Different boundary constraints or developments have been implemented, through the years, on the direct shear apparatus to ameliorate the results and to obtain peak shear strength very close to that of an ideal simple shear. For example, Jewell (1989) proposed the symmetrical arrangement where the top loading platen was secured to the upper half of the shear box. In this arrangement, the out-of-balance moment that tends to rotate the upper frame and the load pad is prevented allowing the loading platen and the upper half of the box to move as a unit throughout the entire test. In the same context, Shibuya et al. (1997) developed another arrangement in which the load pad can be either fixed or point-contacted to the loading piston resulting in a non-tilting mode of motion during the test. Moreover, the opening between the two halves of the box can be maintained at any prescribed value. Lings and Dietz (2004) applied some modifications to the symmetrical arrangement of Jewell (1989) to improve its performance by transmitting the shear load through ball races bearing on wings attached to the sides of the shear box, resulting in what so-called winged DSA (WDSA). In fact, numerous numerical and experimental endeavors have been utilized to examine, in detail, the soil stress and strain development within a shear box. Some of these attempts are listed in Table 1 (Jewell 1989; Zhang and Thornton 2007). The influences of some factors such as the non-uniform deformation and non-coaxiality of principal axes of stress and incremental strain on the interpretation of direct shear test results, discussed by many authors (Jewell 1989; Wang et al. 2007) are also summarized in Table 1.

Based on the brief review of literature on the gradual achievements of data interpretation and DSA development presented in Table. 1, as well as other comprehensive reviews on the subject that have been published elsewhere (Arthur et al. 1997; Gutierrez and Wang 2010), the performance of the physical direct shear apparatus in this study was optimized by exploring modifications to the symmetrical test configuration. This paper re-examines the stresses and

displacements obtained at the DSA boundaries through the three-dimensional (3D) discrete element method (DEM) simulations of physical tests on samples of polydisperse particles using the computer code SiGran (Roubtsova et al. 2011). The balance between the micro-scale change in particle energy and the macro-scale work of external forces is also presented. To achieve confident conclusions about the micromechanics response of samples in direct shear tests, quantitative validations of the DEM models were attempted by relating the physical tests to the corresponding DEM simulations. Experimental direct shear tests were mainly carried out using the symmetrical arrangement suggested by Jewell (1989) and its underlying features described in detail in Appendix A.

Laboratory test procedure

Material

The experimental part of this study was performed using the polydisperse particle standard microspheres produced by Whitehouse Scientific Ltd, England, having the range size of 500-2000 μm each with good sphericity. The particle size distribution, determined by electroformed sieve analysis and the microscopy method, as well as the mechanical and physical properties of selected polydisperse spherical particles are shown in Table. 2.

Shear box testing device and physical testing procedure

In the current study, the performance of the symmetrical direct shear apparatus had been optimized by exploring different test configurations (e.g., fixed load pad to the upper frame, modified collar attachment, initial gap between the shear-box frames, and the use of thin a membrane. A section and plan of the modified symmetrical direct shear apparatus are shown in Figure. 1. The mechanical details of the symmetrical direct shear apparatus are also described in detail in Appendix A. These modifications were suggested by a number of researchers (Jewell

1989; Jewell and Wroth 1987) to ensure the accuracy of results obtained during shearing. The modification that most commonly suggested in these studies is to prevent the load pad and upper frame to rotate during conventional testing.

In the tests conducted here, the polydisperse samples were prepared and sheared in dry conditions. Three direct shear tests were performed at three different normal pressures (50, 200, and 400 kPa) and at a constant relative density of approximately 90%. The maximum and minimum densities of each sample were measured in the dry state using the method specified by Muszynski (2006).

Numerical analysis of direct shear box tests

Theoretical background

The DEM program SiGran used in this study is based on the Discrete Element Method pioneered by Cundall and Strack (1979). An explicit time-stepping numerical scheme is implemented in DEM method to describe the behavior of the assembly of particles interact via a contact logic, and offer a thorough perspective of the response at the particulate level as well as the overall behaviors. The DEM keeps track of the motion of individual particles and updates any contact with neighboring elements according to the Newton's second law. The detailed description of the motion of the particle (i^{th} particle) used in this study is given below (Figure. 2). It worth nothing that, the subscript j refers to the j^{th} neighboring particle, and k is the number of neighboring particles.

$$m_i \frac{d\vec{V}_i}{dt} = m_i \vec{g} + \sum_{j=1}^k (\vec{F}_{cn,ij} + \vec{F}_{dn,ij} + \vec{F}_{ct,ij} + \vec{F}_{dt,ij}) \quad (1)$$

$$I_i \frac{d\vec{\omega}_i}{dt} = \sum_{j=1}^k (\vec{r}_{ij} \times \vec{F}_{ij} + \vec{M}_{ij}) \quad (2)$$

m_i , and I_i are the mass (kg) and moment of inertia (kg.m²) of particle i , respectively. $\vec{V}_i$ and $\vec{\omega}_i$ are the transitional (m/s) and rotational (1/s) velocities of particle i . g is the acceleration of gravity (m/s²) and t is the current time (s).

$F_{cn,ij} = -K_n \delta_n^{\frac{3}{2}}$ (N) is the normal force of contact between particle i and particle j , and δ_n

is the normal contact displacement (m).

$\vec{F}_{ct,ij}$ (N) is the tangential contact force between particle i and particle j , and determined

from numerical integration of $\frac{d\vec{F}_{ct,ij}}{d\delta_t} = -K_t$. $\vec{F}_{ct,ij}$ is limited by the Coulomb's law

$|\vec{F}_{ct,ij}| \leq \mu_s F_{cn,ij}$. δ_t is the tangential contact displacement (m), and μ_s is the sliding friction coefficient, respectively.

$F_{dn,ij} = -C_n \vec{V}_{n,ij}$ (N), and $F_{dt,ij} = -C_t \vec{V}_{t,ij}$ (N) are the normal and tangential damping forces, respectively. $\vec{V}_{n,ij}$ and $\vec{V}_{t,ij}$ are the normal and tangential relative velocities of contact between particle i and particle j .

In equations above, $C_n = 2\sqrt{m^* K_n}$, $K_n = \frac{4}{3} E^* \sqrt{R^*}$, $C_t = K_n \sqrt{\frac{K_t}{K_n}}$, and

$$K_t = 8G^* \sqrt{R^* \delta_n}, \text{ where } \left(\frac{1}{G^*} = \frac{(2-\nu_i)}{G_i} + \frac{(2-\nu_j)}{G_j} \right).$$

The equivalent mechanical and geometrical values marked by stars are defined from values of particles in contact by the following formulas:

$$\frac{1}{m^*} = \frac{1}{|m_i|} + \frac{1}{|m_j|} \quad (3)$$

$$\frac{1}{E^*} = \frac{1-\nu_i^2}{E_i} + \frac{1-\nu_j^2}{E_j} \quad (4)$$

$$\frac{1}{R^*} = \frac{1}{|R_i|} + \frac{1}{|R_j|} \quad (5)$$

where E , ν , G are the Young's modulus (Pa), the Poisson's ratio and the shear modulus (Pa) of particles, respectively. R is the particle radius (m)

$$\vec{T}_{ij} = R_i (\vec{F}_{ct,ij} + \vec{F}_{dt,ij}) \quad (N.m), \text{ and } \vec{M}_{ij} = -\mu_r \left| \vec{F}_{cn,ij} \right| \frac{\omega_i}{|\vec{\omega}_i|} \quad (N.m) \text{ are the rolling torque, and the}$$

friction torque, respectively. μ_r is the rolling (m) friction coefficient.

Input data and simulation process

The simulation were conducted on a polydisperse system of 102248 glass spheres. The same particle size distribution as experimental tests were used for simulations. In DEM models the assigned micro-parameters in the models other than those directly measured were chosen so that to produce the desired macro-properties of the material being tested in the laboratory (Table. 3).

Sample preparation was simulated by placing the particles randomly into the shear box and considering their interaction under the force of gravity. Once the sample was generated, the virtual specimen were subjected to 50, 200, or 400 kPa normal stress. Normal stress was applied as a small displacement at the top boundary. This displacement must be sufficient to stabilize a vertical force after a perturbation of particles at each time step, and small enough to preserve the stability of the numerical solution. In each step, the displacement was calculated using the practical Eq. 6, which takes into account the required normal stress and the diameter of the smallest particle:

$$\delta_v = -1.10^{-3} d_{min} (S_r - S_t) / S_r \quad (6)$$

δ_v is the displacement of the top wall (mm), S_r and S_t are respectively the required and current normal stresses (Pa), d_{min} is the diameter of the smallest particle (mm).

Shearing was imposed by displacing the upper half of the shear box horizontally at a constant velocity equal to that of the experimental tests while the lower half was restrained from moving. The top boundary was free to move vertically, but not to rotate. During all simulations, no out-of-plane motion of upper and lower halves were permitted. The test arrangement adopted for these simulations is schematically illustrated in Figure. 3.

Macroscopic shear test results

In the analysis, virtual and physical samples were all sheared at the same initial relative density and under normal stresses of 50, 200 and 400 kPa. The computed and measured ratios of shear stress to normal stress (τ/σ_n) evaluated at the boundaries at different normal stresses are plotted against the corresponding horizontal displacements in Figure. 4a. It can be seen from Figure. 4a that the peak stress ratio occurs earlier at a relatively low stress level (50 kPa), and the maximum stress ratios decreases with increasing the applied normal stress from 0.65 to 0.57 and from 0.63 to 0.53 for both measured and computed curves, respectively. This reduction in the stress ratio with increasing normal stress is in agreement with earlier results reported by (Ni et al. 2000; Cui and O'Sullivan 2006; Zhang and Thornton 2007) also based on DEM simulations. For all cases examined, Figure. 4a shows also that when the horizontal displacement exceeds a certain limit of 4.5 mm, the stress ratio (τ/σ_n) decreases toward a residual value of about 0.5 at the critical state, irrespective of the initial stress applied.

The computed and measured vertical displacements of the top boundary versus shear displacement are portrayed in Figure. 4b for all cases considered. A positive vertical deflection refers to a decrease in volume, whereas a negative deflection indicates a volume increase. At relatively low normal stress of 50 kPa, dilation of the sample took place at a very early stage of testing. However, when higher normal stress was applied, the virtual samples underwent contractive behavior at the beginning of the test, followed by less significant dilation than that of the lower stress level (50 kPa). For the three numerical cases, the highest dilatancy rate occurs at the peak state, thereafter the rate of dilation decreased with continuous shearing while the critical state was reached. This observation is in agreement with the dilation behavior observed in the experiments. It can be seen that the measured and the calculated peak dilatancy angles deducted from the boundaries measurements underestimate slightly by $\Delta\psi$ less than 2.5° than that inside the shear zone due to averaging effects. The other macro-scale test results are summarized in Table. 4.

Micromechanical analysis

Evolution of anisotropy parameters in fabric

Results of numerous numerical investigations (Cui and O'Sullivan 2006; Bathurst 1985; Thornton 2000) have shown that two competing micro-scale processes take place during the transition to critical state. The first process is a tendency to disorder, which can be observed as a reduction in the coordination number, and corresponding increase in void ratio, e . Superimposed on this process is a tendency to create the anisotropy of fabric and contact forces Bathurst and Rothenburg (1990). The coordination number (CN) is a scalar parameter defined as the mean contact numbers per particle for a granular assembly, where C is the number of contacts, and N is the number of particles.

$$CN = 2C/N \quad (7)$$

Figure. 5a shows the evolution of CN versus the shear displacement for three values of normal stresses. Figure. 5a illustrates that CN decreases rapidly during the initial 8% of the total shear displacement, and flatten off to a relatively steady value while the critical value is attained. In the same context, Figure. 5b shows that CN does not reflect a significant rearrangement of particles, so that the initial reduction in CN values does not attribute to a rapid reduction or increase in density (increase in the absolute value of Δe). In addition, Figure. 5 suggests that higher normal stress value may assist specimen with a larger CN to sustain higher shear stress value in agreement with earlier observations (Cui and O'Sullivan, 2006; Bathurst, 1985; Oda, 1977). However, the coordination number alone is an incomplete description of micro-scale shear deformation, as it carries no information on relative particle orientation and interparticle forces.

Another key parameters controlling the degree of deformation and non-coaxility between principal axes in granular materials subjected to monotonic shearing are the ratio between the degrees of fabric anisotropy and that of force anisotropy, and the angle between the principal fabric direction and the applied loading direction (Bathurst 1985; Rothenburg 1981). These parameters can be quantified by using the data registered during the numerical simulations in the micro-scale. In addition referring to the work by Bathurst and Rothenburg Bathurst (1990), one may use the second-order form of Fourier series expansion to approximate the directional distribution of those micro quantities (Eqs 8-10):

$$E(\theta) = \frac{1}{2\pi} \{1 + a \cos 2(\theta - \theta_a) + b \cos 4(\theta - \theta_a)\} \quad (8)$$

$$\bar{f}_n^c = f_n^0 \{1 + a_n \cos 2(\theta - \theta_n)\} \quad (9)$$

$$\bar{f}_t^c = f_n^0 \{a_w - a_s \sin 2(\theta - \theta_s)\} \quad (10)$$

where the non-dimensional a , a_n , a_s , a_w , and b are coefficients of anisotropy which are measures of the intensity of contact normal $E(\theta)$, normal force $\bar{f}_n^c$, and tangential force $\bar{f}_t^c$ distributions in the directions of anisotropy denoted by θ_a , θ_n , and θ_s , respectively.

Rothenburg (1981) developed powerful relationships, which equate the micromechanical parameters identified above to the macro-scale shear capacity of the system. So that, if distributions for contact force components and contact normal are assumed to have coaxial directions of anisotropy then:

$$\frac{\sigma_t}{\sigma_n} = \frac{1}{2}(a + a_n + a_s) \quad (11)$$

The evolution of fabric anisotropy and contact force anisotropy, i.e. initial, peak, and ultimate states, for the three series of virtual tests are plotted in Figures. 6-8, in terms of the anisotropy magnitudes and directions. The anisotropies of fabric, contact forces during shearing were recorded using a 15 mm high sampling window located at the middle of the box, as shown in Figure. 2. The length of the window was initially equal to the length of the box but was allowed to decrease during the shear process by an amount equal to the shear displacement. After shearing begins, the significant increase in the contact anisotropy is generated primarily by the reduction in the number of contact normal falling within 10 degrees of the minor principal stress direction (Bathurst 1985; Oda and Konishi 1974). Distinctive peaks of number of contacts in θ_a direction represent the higher order chains of contacts extend through the upper left to the lower right corner.

In Figures 6-8, the distribution functions $E(\theta)$, $\bar{f}_n(\theta)$ and $\bar{f}_s(\theta)$ (Eqs. 8-10) appear to well represent the trends of the computed data in all stages. However, unlike approximations using Fourier series, the anisotropies using numerical data do not display full symmetry. This could be interpreted according to Wang et al. (2007) who attributed the asymmetry of the anisotropies to the asymmetry of external loads applied on the shear box boundaries.

Comparing Figures 6-8 shows that the distribution of contact normal at various states are quite similar at different applied normal stresses in that it increases slightly with the increase of the normal stress. This is consistent with the aforementioned observation in Figure. 5 where the larger coordination number achieved at higher normal stress values. On the other hand, it can be seen in Figures 6-8 that although the distribution patterns of normal and tangential contact force are similar, their magnitudes are highly dependent on the applied normal stress.

Normal and tangential contact force distributions during shearing are also shown in Figures. 6-8, so that the evolution of the coefficients of the contact force anisotropy a , a_n , a_s , a_w , and the principal contact force directions θ_a , θ_n and θ_s were obtained from similar plots every 0.5 mm of horizontal displacement and presented in Figure. 9. This Figure shows that the value of a_w is nearly zero and can be eliminated from Eq. 10. Figure 9 shows also a rapid increase in a_n and a_s values at the initial stage of shearing. In the three normal stresses examined, normal and tangential contact force anisotropies reach their maximum values at the peak state. With further shear distortion, the value of a_n gradually decreases while that of a_s fluctuates around a constant value. The orientation of contact normal θ_a and contact force tensors anisotropies θ_n and θ_s are coincided during all stages of the test as illustrated in the lower parts of Figures 9a-c, especially at the peak state. Their minor deviations from coaxiality in other states (stages of shearing) are also negligible, thus Eq. 11 is still valid.

Tracing the anisotropy parameters during the direct shear test, the results of numerical simulations using Eq.11 are shown in Figure. 10 for the three applied normal stresses. These predicted curves appear to be reasonable approximations to the obtained invariant stress ratios from simulations, while the discrepancy is less than 8% at peak state, confirms again the coaxiality of the contact force components and contact normals anisotropies during shearing.

Energy dissipation

The work done by external shear and normal forces must be equal to the change of internal energy contained within the sample. As shown in Figure. 11, for the tested samples under different normal stresses this equilibrium is achieved and the total work applied to the sample increases proportionally with the increase in the applied normal stress.

The internal energy inside the sample consists of different forms of energy which transform from one form to another due to individual particles deformation (elastic energy) and motion (potential and kinetic energies), and their normal and tangential interaction with neighboring particles during an equivalent time step of shearing (Eq. 12). Figure 11 shows that only around 4% of internal energy stored in the system in the form of potential, elastic and kinetic energies, while the majority of the energy dissipated due to the normal and tangential interaction of particles.

$$E_{total} = E_{stored} + E_{dissipated} = (E_{kt} + E_{kr} + E_p + E_e) + (E_{normal-int\ eraction} + E_{tan\ gential-int\ eraction}) \quad (12)$$

where E_{kt} , and E_{kr} are the sum of the translational and the rotational kinetic energies due to

the translational ($E_{kt} = \sum_{i=1}^n \frac{m_i v_i^2}{2}$) and the rotational ($E_{kr} = \sum_{i=1}^n \frac{I_i \omega_i^2}{2}$) motion of all n particles in

the box. E_p is the sum of the gravitational potential energies of all particles ($E_p = \sum_{i=1}^n m_i h_i g$),

where h_i is a position in the height of particle from the bottom of the shear box. E_e is the elastic energy of all individual particles ($E_e = \sum_{i=1}^n (0.5 \cdot \sum_{j=1}^k \int_0^\delta F_{cn} \Delta \delta)_{ij}$).

Two main components of the total internal energy are associated with energies lost through normal and tangential interactions of particles and can be expressed using Eqs. 13-14 Detailed descriptions of the Equations used in the energy analyses presented here can be found in Roubtsova et al. (2015).

$$E_{normal-interaction} = E_{dn} = \sum_{j=1}^k \left(\int_0^\delta F_{dn} \Delta \delta \right)_{ij} \quad (13)$$

$$E_{tangential-interaction} = E_f + E_{dt} - E_M + E_{Md} \quad (14)$$

$$= \sum_{j=1}^k \left(\int_0^{\delta_t} F_{ct} \Delta \delta_t \right)_{ij} + \sum_{j=1}^k \left(\int_0^{\delta_t} F_{dt} \Delta \delta_t \right)_{ij} - 0.5 \left(\sum_{j=10}^k \int_0^\varphi r_i (\bar{F}_{ct} + \bar{F}_{dt}) \Delta \varphi \right)_{ij} + \left(\sum_{j=10}^k \int_0^\varphi M_{di} \Delta \varphi \right)_{ij}$$

In these equations, k is the number of contacts for particle i with neighboring particles j . E_{dn} and E_{dt} are the energies dissipated from the system by damping through the moving of particles respectively in the normal and the tangential directions. E_f is the energy that dissipate when one particle slide on another in the present of friction. E_M is the work of moments because of friction and dissipation forces that saved by the system, while, E_{Md} is the work of dissipation moment. φ is a relative angle of rotation of particles during interaction (rad).

The variation of energies associated with dissipation during the normal and the tangential interactions of particles versus shear displacements are portrayed in Figure. 11 for the three virtual tests. The ratio of the averaged consumed energy associated with the normal and the tangential interaction of particles to the total internal energy are 28%, 39% and 41%, and 68%,

57% and 55%, respectively for normal stresses of 50 kPa, 200 kPa, and 400 kPa. Figure. 12 shows that at normal stress of 50 kPa the energies dissipated through the tangential interaction of particles at contacts are maximum in a shear plane, while the energies associated with the normal forces at contacts distribute along the diagonal of the shear box. Same trend was also observed for other applied normal stresses during shearing.

In Figure. 13, the amount of consumed internal energy contributes to the dilation of sample has been calculated and portrayed versus shear displacements for the three virtual tests. The increase of dilation energy, with increasing applied normal stress is apparent in this Figure. Comparing the dilation energy curves with their corresponding vertical displacements shows the initiation of negative dilation energy is consistent with the compression of the sample at the beginning of shearing. Thereafter, the dilation energy gradually increases and approaches the constant value at the shear displacement corresponding to the point of zero rate of dilation and complete shear band formation.

In Figure. 14, the energy attributed to the rotation of particles is shown as a component of the tangential energy at contacts. As shown in this Figure, the average rotational energy consumed inside the sample is practically small within the whole specimen, less than 6% for the three cases. In other words, the internal energy dissipated through the tangential interaction of particles can be mainly attributed to the sliding of particles.

Although the amount of rotational energy is small compared to the other components of tangential energy at contacts., it can be viewed as a good indicator of shear localization leading to the establishment of shear bands (Jewell and Wroth 1987; Potts et al. 1987; Zhang and Thornton 2007; Dyer and Milligan 1984; Oda and Kazama 1998). Figure. 15 presents the spatial distribution of rotational energy inside the samples together with the rotational energy along

their heights during different stages of shear distortion (O-A, A-B, B-C, and B-D). During stage O–A (start of shearing), the rotational energy at the mid-height of the sample starts to increase. However, the rotational energy is relatively small compared to its counterparts at later stages and its distribution is not presented in Figure. 15. It should be noted that in stage A-B (start of dilation), the resolution of rotational velocities is two times greater than that used for other stages, in order to visualize the formation of shear band clearly at all stages. Stage A-B corresponds to the strain localization at the two lateral boundaries, owing to the boundary constraint. As shearing proceeds, the shear zone extends slowly toward the middle of the box from the boundaries. At stage B-C (peak state), a distinct shear band has been formed over the length of the middle plane, where the rotational energy becomes more pronounced. As more shear deformation is applied, the rotational energy becomes more significant for the particles inside the central shear zone than the particles outside. This is the stage where the upper half of the shear box and particles are subjected to the uniform block-like motion (Stage C-D). The spatial distributions of rotational energy during shearing is consistent with the dispersion of individual particles rotation found in other studies (Ni et al. 2000; Zhang and Thornton 2007; Bardet 1994), describing the extent of uniform shear zone located at the mid-height of the specimen. This Figure reveals that the increase of rotational energy for all three samples are confined to the zone around $10 D_{50}$. In addition, According to some studies (Oda and Kazama 1998; Arthur 1988), the localization of the shear band is mainly characterized by the formation of the extremely large voids which caused by the large dilatancy taking place inside the shear zone. Amirpour Harehdasht et al. (2017) showed, in agreement with this study, that the increase of the void ratio in within the simulated samples during direct shearing is confined to the zone equal to $10\text{--}12 D_{50}$, with the peak at the mid-plane of the box, while remains unchanged close to the top and bottom boundaries during the shearing.

Verification of the Peak Plane Strain Friction Angle

The two possible orientations suggested for the shear band at peak state are along planes of maximum mobilized strength based on the Mohr-Coulomb failure criterion or along the direction of the zero linear extension (Skinner 1969). According to (Arthur et al. 1988; Dyer 1985) owing to the degree of constraints imposed on the sample in direct shear test, soil may have no choice but to develop along the zero-extension direction and satisfy Roscoe's solution. However, the Mohr-Coulomb solution yields the upper-bound value of orientations measured from the horizontal (Table. 4). The shear band orientation predicted from the Roscoe equation justifies the assumption of horizontal zero linear extension direction made at peak state, where the deviation of the zero linear extension direction from the horizontal at the peak state is less than 1.15° for the three numerical cases examined.

Assuming uniform deformation inside the shear band, coincidence between principal axes, and horizontal zero linear extension direction, the plane strain frictional shearing resistance of the sand can be derived from the geometry of Mohr's circle (Davis 1968):

$$\sin \phi_{ps} = \frac{\tan \phi_{ds}}{\cos \psi (1 + \tan \psi \tan \phi_{ds})} \quad (15)$$

Nevertheless, the plane strain angle of friction interpreted from this equation would be in error due to the underestimated angle of dilation evaluated at the boundaries, deviation of the zero linear extension from horizontal, or non-coaxiality between the principal axes of stress and incremental strain. Jewell (1989) and Wang et al. (2007) extended Davis's relation to take full account of these conditions. An extended relationship based on Wang et al. (2007) is used

herein to account for the non-coaxiality of principal axes and the deviation of the zero linear extension direction from horizontal:

$$\sin \phi_{ps} = \frac{\tan \phi_{ds}}{\cos(a - 2\Delta\theta) + \sin(a - 2\Delta\theta)\tan \phi_{ds}} \quad (16)$$

where $\Delta\theta$ is the non-coaxial angle and a is a geometrical angle derived from the Mohr's circle of incremental strain as $d\nu$ and $d\gamma$ are invariants of volumetric and shear strain increment:

$$\sin a = \frac{d\nu/2 - d\epsilon_{yy}}{d\gamma/2} \quad (17)$$

A slight difference, less than 1° , between the plane strain angle of frictions using Eq. 15 and Eq. 16 presented in Table. 4 reveals the minor effect of non-coaxiality in the three numerical cases at peak states. These observations, in full agreement with Jewell and Wroth (1987) and Wang et al. 2007, verify the precision of the stresses and displacements evaluated at the boundaries of direct shear apparatus where the symmetrical arrangement Jewell (1989) is implemented.

Conclusions

The prime objective of this study was to analyze the macro and micromechanics behavior of granular material (polydisperse particles) tested in symmetrical direct shearing as suggested by Jewell (1989) by means of three-dimensional (3D) discrete element method (DEM). The numerical results were compared to their experimental counterparts at the macro-scale under different applied normal stresses. The balance between the micro-scale change in particle energy and the macro-scale work of external forces as well as the coaxiality between the principal stresses and the principal strains increments directions are discussed. The following conclusions can be drawn from this study:

1. The evolution of the shear stress to normal stress ratio (τ/σ_n) and the boundary dilation angles obtained from DEM simulations are almost similar to those inferred from the boundary calculations of the physical tests. However, the values of the dilation angles inside the shear zone of the virtual samples are slightly greater than the boundary dilation angles.
2. The distribution of the contact normal and the contact forces exhibits the same evolution patterns of anisotropy under different applied normal stresses. However, significant discrepancies are noted in the distributions of the magnitude of the normal and the tangential contact forces.
3. There is a good agreement between the approximated (τ/σ_n) curves obtained from the anisotropy parameters and the stress ratio from the boundaries of the virtual samples, which confirms the coaxiality of the contact force components and contact normal anisotropies during shearing.
4. The numerical results show that the energy transmitted by the external forces to the sample consumed primarily by the normal interaction of particles as well as their relative movements through rolling and sliding. Although the ratio of the rotational energy to the tangential energy is less than 3%, it is still an indication of the strain localization.
5. The micro-scale results show that the strain localization initiates from the boundaries and extends towards the middle of the shear box while developing a continuous and uniform shear band along the middle plane of the box. Correspondingly, rotational energy localizes within the shear zone whereas it steadily increases with the shear deformation.
6. The slight difference between the plane strain friction angles calculated from the conventional Davis's equation (Davis 1968) and those obtained from the extended equation of Wang et al. (2007) accounting for the non-coaxiality behavior as well as the deviation of

zero linear extension direction, confirms again the minor effect of the non-coaxiality at the peak state.

The results presented in this paper suggest that the measurements at the boundaries of the symmetrical direct shear test are quite appropriate for determining strength and volume change behavior of granular soils.

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Table 1. Examples of DSA experimental and numerical previous investigations.

Author(s)	Type of work	Main findings
Jewell & Wroth (1987)	Experimental study Symmetrical arrangement 'induced' rotational restraint	<ul style="list-style-type: none"> Uniform band of deforming sand is generated across the sample center. The deviation of the zero linear extension direction at peak state from the horizontal is negligible.
Potts et al. (1987)	Numerical simulation 2D FEM	<ul style="list-style-type: none"> The strains and stresses within the failure zone at the peak are uniform. Progressive failure effect is found to be minor within the final failure zone.
Jewell (1989)	Experimental study Symmetrical arrangement	<ul style="list-style-type: none"> Symmetrical DSA results correspond closely to those in the simple shear for both ϕ_{ps} and ψ. Non-uniform deformation and non-coaxiality behavior can be considered to interpret DSA results.
Shibuya et al. (1997)	Experimental study 'enforced' rotational restraint	<ul style="list-style-type: none"> Nonrotating loading platen is needed to optimize the results. Effect of wall friction and membrane are not pronounced in a symmetrical arrangement.
Ni et al. (2000)	Numerical simulation 3D DEM (PFC ^{3D})	<ul style="list-style-type: none"> The major deformation of each sample is located within a narrow shear zone at its mid-height.
Masson & Martinez (2001)	Numerical simulation 2D DEM	<ul style="list-style-type: none"> The shear process induces a clear change in contact and contact force orientations. There is a correlation between the induced anisotropy of the microstructure and macroscopic loading.
Lings & Dietz (2004)	Experimental study The Winged DSA (WDSA)	<ul style="list-style-type: none"> Symmetrical arrangement (Jewell 1989) is recommended to adopt in routine direct shear tests. Upper-frame rotation has an almost negligible effect on the measured parameters in symmetrical tests.
Cui & O'Sullivan (2006)	Numerical simulation 3D DEM	<ul style="list-style-type: none"> Significant stress and strain non-uniformities exist within specimens undergoing direct shear tests. Shear stresses calculated along the boundary are lower than those calculated close to the mid-height.
Wang et al. (2007)	Numerical simulation 2D DEM (PFC ^{2D})	<ul style="list-style-type: none"> The effect of non-coaxiality is minor for granular material at peak state. Deviation of zero linear extension direction from the horizontal at peak state is small. The strength and volume change behavior evaluated at the boundaries of the DSA are valid.
Zhang & Thornton (2007)	Numerical simulation 2D DEM	<ul style="list-style-type: none"> The principal directions of stress and strain-rate are coaxial under steady-state conditions. Evolution of stress ratio inside the shear band is similar to that inferred from boundary forces.

than that obtained from the boundary observations.

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Table 2. Properties of polydisperse spherical particles

500-2000 (μm)	Size at Fixed Percentiles (μm)							
	1	5	10	25	50	75	90	95
Final Mean Size (μm)	524	623	691	853	1011	1248	1534	1687
(+/-) 95% confidence	3.2	4.9	5.7	7.8	11	24	48	38
Mechanical/ Physical Properties	Young Modulus (N/mm^2)				6.89×10^4			
	Rigidity Modulus (N/mm^2)				2.96×10^4			
	Poisson ratio				0.21			
	Specific Gravity (gr/cm^3)				2.43-2.49			

Table 3. Input Micro-Parameters for DEM simulations

Parameter	Value
Young’s Modulus	68.9 GPa
Poisson Ratio	0.21
$e_{max} - e_{min}$	0.69- 0.51
Density	1603 kg/m ³
Coefficient of sliding friction particle-particle	0.2
Coefficient of sliding friction wall-particle	0.3
Coefficient of rolling friction	5.10 ⁻³ mm

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Table 4. Peak and critical state strength ratios and dilation angles evaluated by experimental tests and numerical simulations

Parameter	$\sigma_n = 50kPa$	$\sigma_n = 200kPa$	$\sigma_n = 400kPa$
Experimental Tests			
Peak $(\tau/\sigma)_{ds}$ ¹	0.65	0.58	0.57
Peak ϕ_{ds} (°) ²	32.96	30.14	29.66
Peak ϕ_{ps} (°)-Eq. (15) ³	34.19	31.50	31.08
Critical State ϕ_{ds} (°)	28.23	26.56	25.96
Peak ψ (°) ⁴	18.50	14.13	13.10
Numerical Simulations			
Peak $(\tau/\sigma)_{ds}$	0.63	0.60	0.53
Peak ϕ_{ds} (°)	32.45	31.09	28.05
Peak ϕ_{ps} (°)-Eq. 15	33.48	32.34	29.06
Peak ϕ_{ps} (°)-Eq. 16	33.61	31.36	29.29
Critical State ϕ_{ds} (°)	27.06	25.54	24.21
Peak ψ (°)	19.07	14.30	13.50
Peak $\Delta\theta$ (°) ⁵	-1.28	-3.00	0.00
Peak $\Delta\psi$ (°) ⁶	0.85	2.30	1.50
Orientation of Shear band			
Mohr-Coulomb (°)	7.74	7.32	8.53
Roscoe (°)	0.53	1.15	0.75

Note:

¹ τ is the average horizontal shear stress; σ is the average vertical normal stress² $\phi_{ds} = \tau/\sigma$ is the direct shear friction angle³ ϕ_{ps} is the plane strain friction angle⁴ $\psi = d\nu_y/d\nu_x$ is the dilation angle measured in boundaries, where $d\nu_y$ and $d\nu_x$ are the rate of change of vertical and horizontal displacement, respectively.⁵ $\Delta\theta$ is the angle between principal stress and principal strain incremental directions⁶ $\Delta\psi$ is the difference in the computed dilation angle in boundaries to that inside the shear band

<https://mc06.manuscriptcentral.com/cgi-pubs>
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APPENDIX A: Mechanical details of the symmetrical direct shear apparatus adopted for this study

In symmetrical direct shear test, the sample is contained within a shear box, and confined between a retaining plate and load pad. The steel shear box, square in plan, is split horizontally at mid height, forming an upper and lower frame. The features of the apparatus are as follows:

- a) *Sample geometry*: The specimen is square in plan, with a length and width of 55 mm.
- b) *Symmetrical arrangement*: The modifications and suggestions proposed by [16, 19] were implemented in the direct shear apparatus to achieve the so-called symmetrical arrangement. They proposed the load pad to be fixed to the upper frame, where there would be no out-of-balance moments tending to cause rotation. According to [16] the moment created by the lever arm between the horizontal forces is exactly balanced by the moment created by the eccentric vertical force acting on top of the sample in a symmetrical arrangement. Using radiography technique and dial gauges to measure lateral tipping and horizontal rotation, [16] proved there is no tendency for either to occur in a symmetrical arrangement.
- c) *Shear Load*: Shear load is applied to the apparatus in the displacement-controlled fashion at a constant velocity of 0.0051 mm/s, driven by an electric motor. The shear load applied at the level of the mid-plane of the sample and is transmitted to shear box by a rigid connector **A**.
- d) *Roller bearings*: The direct shear carriage is mounted on freshly cleaned and lubricated two tracks of rollers **F**, which allow free movement in the direction of shear and prevent any lateral movement. The lower half of the box fit firmly into the shear box against the spacer blocks at the driving end of the carriage.
- e) *Normal load*: The loading piston **B** is point contacted to the load pad, which results in not-tilting modes respectively [16, 19]. The vertical load applied directly to the top piston using a system of an air compressor attached to a lever, and is kept constant during testing.

- f) *Collar attachment*: Unlike the conventional arrangement, where locked collar attachment **C** prevents vertical displacement and creates clockwise moment on the upper half; the arrangement of the collar attachment **D** in using apparatus ensures freedom of vertical movement with no induced friction and momentum, so that dilation can take place unimpeded.
- g) *Gap size*: Researchers suggested the initial gap between the upper and lower halves of the shear box, so that the whole of the horizontal shear force can be transmitted through the specimens itself. Head [47] suggested a gap lightly more than the diameter of the largest particles. Jewell [16] recommended 0.5 mm opening between the upper and lower halves. Similarly, [48] recommends a standard value of 0.64 mm gap size for tests on fine sands. [18] recommended a gap size of $5D_{50}$ for direct shear tests on Leighton Buzzard sand (Rounded particles, $D_{50}=780\ \mu\text{m}$). However, they also mentioned that there would be a range (between 2 mm to 4 mm), where identical results of both peak friction and peak dilation angles were recorded. In this study, the direct shear test results with different gap sizes of 0.5 mm, 2 mm, 4 mm and 5 mm were compared, and the gap size of 2mm was adopted. Peak friction and peak dilation angles varied by 5° for the range of gap sizes investigated. The small gap of 0.5 mm showed enhanced friction and dilation angles up to 4° , and preventing the probable contraction of samples at the beginning of the test. The peak friction and dilation angles were similar for both gap sizes of 4 mm and 5 mm. Samples with gap size of 2 mm showed the maximum difference just over 1° compare to samples with larger gap size. In addition, compared to samples with larger gap size no unintended jamming of the membrane and escape of material into the gap occurred during sample preparation and shearing for adopted gap size of 2 mm.
- h) *Edging*: During the shearing, especially when the sample dilated excessively, the collapse of the material at the edges might occur and assist a progressive failure mechanism. The outflow of the sample would increase the moment during shearing and cause the upper shear box and the top plates to tilt. A supplementary split membrane of thin latex **E** was therefore laid over the interior

walls of the frames, to prevent the sample from flowing out. This technique has been used previously [17, 18, 49], showing the effect of membrane expected to be not the problem for the symmetrical type of shear box used in this study [17]. This is in agreement with our observations for samples with small gap size of 0.5 mm, where outflow was minor and the effect of the membrane on shearing behavior seemed practically negligible. These samples showed nearly constant volume soon after reaching the maximum shear strength, and the failure envelopes nearly coincide for samples with and without the membrane.

- i) *Mechanical details:* Further details of the direct shear can be seen in Figure. 1, showing using thick rubber **G** secures the load pad in symmetrical tests from rotation. The two halves are temporary fixed together by means of two clamping screws **H**, which have to be removed before proceeding to the shearing stage. The comprehensive arrangement of lifting spacers **I** is used to pre-set the gap between the frames. Lifting spacers have to be removed carefully before applying the normal force.