Exploring the relationship between particle shape and critical state parameters for granular materials using DEM

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Abstract

This paper establishes the relationship between particle shape and critical state parameters for granular materials using discrete element method (DEM). A series of DEM simulations are performed under drained triaxial test conditions considering a varying elongation parameter (η). The elongated particles are generated using a commonly employed multi-sphere approach. From the analysis of results, it is found that the macroscopic response of elongated particles exhibits post-peak strain-softening behaviour while reaching a critical state at an axial strain of $\sim 40\%$. The critical state strength of granular materials is found to be dependent on η . The microscopic behaviour in terms of coordination number (CN) shows an exponential decay against axial strain. In the early stage, CN decreases with increasing η , while the steady-state CN is found to increase with an increase in η values. Furthermore, quantitative relationships are established among the shape parameters and critical state parameters, thus providing a way to develop macro-scale constitutive models with intrinsic micro-scale built-in properties of granular materials.

Keywords DEM · Triaxial test · Critical state · Particle elongation · Shape parameters

1 Background

Most geomaterials are comprised of individual discrete particles which interact with each other at microscopic contacts to sustain any external loads imposed on them. These materials behave differently in comparison to regular solids and exhibit many important behaviours such as dilatancy, anisotropy and nonlinearity [51]. The response developed by contact interactions depends on particle shapes to a large degree. Thus, the particle shape of granular materials needs to be systematically varied so that quantitative relations between shape parameters and critical state properties for these materials may be discovered.

Numerous studies have shown that particle features have well-known effects on the characteristic behaviour of granular materials, including strength of the particle [23,

37, 47], size of the particle [9, 12, 43, 54, 56], particle size distribution [9, 20, 25, 31, 39, 46, 48] and shape of the particle [2, 6, 51]. Recently, research interest has been growing on exploring the particle scale characteristics of granular materials considering an in-depth understanding of the microscopic parameters (e.g. [5, 19, 40, 52]).

Multiple definitions of representative shape parameters which can be used to describe the shape of particles may be found in the literature (e.g. [10, 11, 17, 24, 52, 51]). Among the various grain shape parameters, particle size and gradation are commonly used in soil mechanics. In contrast, due to the involvement of sophisticated equipment and the difficulty involved in laboratory grain-scale measurements, very limited progress has been made in the literature on quantifying the effects of particle shape characteristics of granular

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materials. Alternately, DEM based investigations are useful in understanding the particle shape characteristics of granular materials as evidenced by Gong and Liu [13] and Kodicherla et al. [18].

An experimental study by Xiao et al. [49] found that all the samples at an initial relative density of 0.6 exhibited strain-softening and volume-expansion behaviour. The slope of the relationship between the peak-state friction angle and maximum dilation angle was independent of the particle shape, whereas the intercept was significantly influenced by particle shape. Yang and Luo [51] explored the relationship between critical state and particle shape for granular materials and found that the mixture of Fujian sand and spherical glass beads was found to be markedly more susceptible to liquefaction than the mixture of Fujian sand and crushed angular glass beads.

The core idea of this article is to establish the relationship between particle shape and critical state behaviour of granular materials. A series of drained three-dimensional triaxial test simulations are performed considering different values of the dimensionless elongation parameter (η). At the onset, the evolution of macroscopic behaviour is explored and then the behaviour of the micro-scale response considering coordination number (CN) and deviator fabric (ϕ_d) is discussed. Finally, the relationship between the particle shape and critical state parameters of granular materials is established.

2 Methodology and shape characteristics

The elongated particles are generated as a juxtaposition of three independent spheres of radius R' with an imaginary rectangle of length L and width $2R'$. Assuming that R is the radius of a circle circumscribing the particle, the radius R' is also that of the inscribed circle. A dimensionless elongation parameter, η , is defined as:

$$\eta = \Delta R / R \quad (1)$$

where ΔR is the deviation from the circular shape which is equal to half of the length (L) of the imaginary rectangle. The elongated particles are modelled using a commonly adopted multi-sphere (MS) approach, as suggested by [41]. More details on the particle generation approach can be found at [3, 19]. For the analysis, we employed a commercially available package called particle flow code (PFC) developed by Itasca Consulting Group [16].

In general, particle shape can be characterized by three shape parameters, i.e. aspect ratio (A_R), convexity (C_X) and sphericity (S_W) [4, 21, 22, 32, 44]. The definitions of these shape parameters are given as:

- Aspect ratio (A_R): The ratio between minimum Feret diameter ($D_{\min}^F$) and the maximum Feret diameter ($D_{\max}^F$).

$$A_R = \frac{\text{Diameter}_{\min, \text{Feret}}}{\text{Diameter}_{\max, \text{Feret}}} = \frac{D_{\min}^F}{D_{\max}^F} \quad (2)$$

- Convexity (C_X): The measure of the compactness of a particle. In three dimensions, it can be evaluated as the ratio between the particle volume, V_p and the volume of the particle's convex hull, V_{CH} .

$$C_X = \frac{\text{Volume}_{\text{particle}}}{\text{Volume}_{\text{Convex hull}}} = \frac{V_p}{V_{CH}} \quad (3)$$

- Sphericity (S_W): The measure of how closely a particle resembles a sphere. According to [44], it is the ratio between the surface area of a sphere which is believed to have the same volume and surface area of that particle.

$$S_W = \frac{\pi^{1/3} (6V_p)^{2/3}}{S_p} \quad (4)$$

where V_p and S_p are the volume and surface area of a particle, respectively. The range of S_W varies from 0 to 1 ($0 < S_W \leq 1$), with 1 being that of a spherical particle.

Overall regularity (O_R): It represents the impact of these three-particle shape parameters (i.e. A_R , C_X and S_W) in an integrated manner, considering the fact that the geometry of a particle tends to be more round and regular as each of the three shape parameters increases, which can be indicated by the definitions of the three parameters (A_R , C_X and S_W) and is shown by [51].

$$O_R = \frac{(A_R + C_X + S_W)}{3} \quad (5)$$

It should be noted that A_R , C_X , S_W and O_R can only reflect the shape characteristics of a particle but not the whole granular assembly. The generated elongated particles with varying shape parameters are presented in Fig. 1.

3 Simulation details

The three-dimensional triaxial test specimen is modelled using six independent rigid walls comprised of a cubic box with dimensions of $5 \times 5 \times 5$ cm. In view of the computational expense and literary suggestion, each assembly is restricted to 2845 clumps made up of about 8535 pebbles. According to Ng [28], if the number of particles lies in between 1170 and 3000, the boundary effects of the assembly can be neglected. Similar potential effects of

Fig. 1 Elongated particles with varying shape parameters

Table 1 Basic characteristics and shape parameters

Elongation parameter (η)	Initial void ratio (e_0)	Initial coordination number (CN_0)	A_R	C_X	S_W	O_R
0.1	0.52	13.4	0.90	1.000	0.997	0.966
0.2	0.46	12.0	0.80	0.999	0.988	0.929
0.3	0.45	11.7	0.70	0.997	0.971	0.889
0.4	0.45	11.6	0.60	0.991	0.941	0.844
0.5	0.49	11.4	0.50	0.976	0.890	0.789
0.6	0.59	11.3	0.40	0.932	0.800	0.711

particle numbers on simulation results were also observed by [15] and Wang and Gutierrez [45]. A random seed generator is used to distribute the particles randomly and no gravity is applied to the particles. The basic characteristics of the assemblies used are presented in Table 1.

A simple linear force–displacement contact law is implemented to mimic the clump-clump and clump-wall interactions [1, 15, 19, 38, 50, 53]. For isotropic compression, an in-built servo-mechanism is activated to maintain the desired stress levels within the assembly. While shearing, both the top and bottom walls are permitted to move towards each other at a constant loading rate of 0.004 m/s, whereas the remaining walls maintain the same confining pressure using a stress-controlled servo mechanism [55]. In addition, auto time-step scaling mode in PFC is enabled

Table 2 Input parameters for DEM simulations

Parameter description	Value
Notional particle density, ρ (kg/m^3)	2700
Inter-particle friction coefficient	0.5
Wall-particle friction coefficient	0.0
Wall stiffness (N/m)	1.0×10^9
Effective modulus, E^* (Pa)	1.0×10^8
Normal to shear stiffness ratio, $k^* (\equiv k_n/k_s)$	4/3
Local damping constant	0.7

to reduce the computational time with associated DEM simulations [8]. The basic input parameters used are presented in Table 2.

4 Results and discussion

The mechanical behaviour of the granular assembly during shear can be evaluated by a stress tensor. It is evaluated based on the average volume of contact forces, which is given as [7]:

$$\sigma = \frac{1}{V} \sum_{c \in V} f^c \otimes l^c \quad (6)$$

where V is the total volume of the assembly; f^c is the contact force vector at contact c ; l^c is the branch vector joining the centres of the two contacting particles at contact c ; $\otimes$ is the dyadic product. The two commonly used invariants of σ , the mean effective stress p and deviator stress q , are given as:

$$p = \frac{1}{3} \text{tr} \sigma \quad (7)$$

$$q = \sqrt{\frac{3}{2} \text{dev}(\sigma) : \text{dev}(\sigma)} \quad (8)$$

The deformation of a specimen is quantified by the axial strain ε_z and the volumetric strain ε_v from the displacements of the rigid walls (boundaries), i.e. $\varepsilon_z = \ln(H_0/H)$, $\varepsilon_v = \ln(V_0/V)$, where H and V are the height and volume of the specimen during shearing, respectively. Similarly, H_0 and V_0 are the initial height and volume of the assembly. It should be noted that all samples are isotropically compressed to 200 kPa (unless otherwise mentioned).

4.1 Macroscopic behaviour

For the evolution of η on the macroscopic behaviour of granular materials, all assemblies are generated at their densest state inputting an internal friction coefficient of zero during the sample preparation phase. This approach has also been adopted by several investigators (e.g. [13, 19]). Figure 2 shows the evolution of stress ratio (q/p) against axial strain for different values of η . All specimens exhibit similar behaviour, i.e. post-peak strain-softening, which is commonly expected in the dense granular assemblies. Furthermore, the stress ratio flattens off and tends to follow a steady-state after an axial strain of 40%, which is said to have reached a critical state [14, 36]. Similar observations were also observed by [19], for the DEM simulations of the direct shear test.

The mobilised shear strength of the granular assembly during the triaxial shear test is represented by the angle of internal friction ϕ' , which is given as:

$$\phi' = \arcsin \left\{ \frac{\sigma'_1 - \sigma'_3}{\sigma'_1 + \sigma'_3} \right\} = \arcsin \left\{ \frac{3q/p}{q/p + 6} \right\} \quad (9)$$

where σ'_1 = major principle effective stress; σ'_3 = minor principle effective stress. The effect of η on the angle of internal frictions at both the peak and critical states is presented in Fig. 3. The peak state is recognised as the state at which the stress ratio reaches a peak value against axial strain, whereas the critical state is considered to be the one at which the granular assembly is continuously sheared

Fig. 2 Stress ratio against axial strain for different η

Fig. 3 Effect of η on the angle of internal frictions

under constant volume and stresses. The error bars represent the standard deviation of the friction angles at a critical state. As can be seen from Fig. 3, the peak state friction angles reached a peak value at $\eta=0.2$ and almost stabilized with further increases in η . In general, the critical state friction angles increase with the increase in η . According to Gong and Liu [13], as aspect ratio increases, the value of peak state friction angles exhibits a unimodal peak, whereas the critical state friction angle is monotonically increased. Although the same approach (i.e. MS approach) was used in both investigations, the variations in both peak and critical state friction angles are identified. These findings do not match those of the current investigation; this might be due to the different initial conditions and the number of spheres in each clump.

Figure 4 illustrates the effect of confining stresses on the triaxial shear behaviour of granular materials for $\eta=0.3$. All assemblies reach the critical state at the same critical state stress ratio (i.e. stress ratio of q/p with a value of 1.0), which indicates that the residual shear strength of the assemblies is independent of the applied confining stress. However, the peak stress ratio of the assemblies with different confining stresses is slightly varied. These findings are in agreement with the studies conducted by Gong and Liu [13] and Kodicherla et al. [19]. The generated ellipsoids using the MS approach

have multiple contacts resulting in stronger interlocking, enhancing the shear strength of the granular assembly. In the case of true ellipsoids, the effect of interlocking may be limited because of the smooth surface; consequently, lesser shear strength was achieved [29].

Figure 5a shows the evolution of volumetric strain against axial strain for different η values. It is observed that all assemblies exhibit initial contraction and then continuous dilation until reaching the critical state. Moreover, it is seen that η has a significant impact on the volumetric behaviour of granular assemblies. For instance, the sample with $\eta=0.1$ reaches a critical state of about 30% of axial strain, whereas for the case $\eta=0.6$, about 45% of axial strain is required to reach the critical state. The values of void ratio (e) initially decrease up to $\eta=0.3$ but increase with further increases in η (Fig. 5b). This observation is somewhat different from the behaviour of granular materials obtained using the MS approach by Gong and Liu [13]. This might be due to the method of particle generation which has a marked influence on the spatial arrangement and the critical state void ratio (e_c) of granular assemblies. The relationship between void ratios and η at different stages of axial strain is shown in Fig. 5c. The values of e reach a minimum value at $\eta=0.4$, and they increase with the increase in η for different percentages of axial strains.

Fig. 4 Stress ratio against axial strain for different isotropic stresses

Fig. 5 **a** Evolution of volumetric strain against axial strain; **b** evolution of void ratio against axial strain; **c** relationship between void ratio against η at different stages of axial strains

4.2 Microscopic behaviour

4.2.1 Coordination number (CN)

The CN is a fundamental microscopic parameter, which can provide the structural stability of a granular assembly [34, 42]. In a simple form, the CN is defined as the average number of contacts per particle. Figure 6 presents the evolution of CN against axial strain for different η values. All samples follow an exponential decay against the axial strain. The inset (Fig. 6) shows the initial and steady-state CN of the assemblies with different η values. In the very early stage, CN decreases with increasing η while the steady-state CN is found to increase with the increase in η values. This may be due to the variation in η and the consequent contact interactions while shearing the assembly.

According to [30], the fabric is used to describe the spatial arrangement of particles. There exist different definitions for the fabric tensor (e.g. [26, 30, 35]). However, a contact-normal-based fabric tensor is commonly adopted to investigate the spatial arrangement of particles during shear (e.g. [30, 35]).

$$\phi_{ij} = \frac{1}{N_c} \sum_{k=1}^{N_c} n_i^k n_j^k = \begin{bmatrix} \phi_{11} & \phi_{12} & \phi_{13} \\ \phi_{21} & \phi_{22} & \phi_{23} \\ \phi_{31} & \phi_{32} & \phi_{33} \end{bmatrix} \quad (10)$$

where n^k is the contact unit normal vector of the contact k with $i, j = 1, 2, 3$ and N_c is the number of contacts in the assembly. The components ϕ_{11} , ϕ_{22} and ϕ_{33} indicate the

average orientation of contacts which is distributed uniformly in the x , y and z directions, respectively. The scalar values of the shear components in the opposite direction are equal, that is, $\phi_{12} = \phi_{21}$, $\phi_{13} = \phi_{31}$ and $\phi_{23} = \phi_{32}$. The principal values ϕ_1 , ϕ_2 and ϕ_3 along the principal directions of fabric can be evaluated using the eigenvalues and eigenvectors of the fabric tensor. The deviator fabric, $\phi_d (= \phi_1 - \phi_3)$, is the difference between the major and minor principal fabric components, which is widely used to quantify the structural anisotropy of granular assemblies [42]. The evolution of deviator fabric against axial strain for different η values is shown in Fig. 7. The deviator fabric at small strains mainly depends on both the stress and volume change, while at large strains, the volume approaches a steady value and the deviator fabric depend only on the stress [19]. Thus, the trend of ϕ_d also follows as same as the behaviour of stress–strain response as shown in Fig. 2.

4.3 Relationships between critical state and shape parameters

In soil mechanics, it is well known that the critical states are attained at large shear strains as a straight line in the given stress space with an effective stress ratio M :

$$q = Mp' \quad (11)$$

where q is the deviator stress and p' is the mean effective stress. In the $e - p'$ space, the locus of critical states is often described by a linear function given by [33, 36] as:

Fig. 6 CN against axial strain for different η

Fig. 7 Evolution of deviator fabric against axial strain for different η

$$e = e_c = \Gamma - \lambda \log p' \quad (12)$$

where e is the void ratio; e_c is the void ratio at the critical state; λ is the slope of the straight line; and Γ is the void ratio intercept (i.e. typically taken as $p' = 1$ kPa). A method to linearize the critical state line (CSL) in the $e - (p'/p_a)^\xi$ space is given as [27]:

$$e = e_c = e_\Gamma - \lambda_c \left(\frac{p'}{p_a} \right)^\xi \quad (13)$$

where p_a is the atmospheric pressure ($= 101.325$ kPa) which is used for normalization; e_Γ is the void ratio at intercept $p' = 0$, and λ_c is the slope of the CSL, and ξ is a material constant parameter, which is taken as $\xi = 0.7$, for standard Toyoura sand [27] and in the relevant DEM simulations [13, 19].

The CSL may change its position by the transformation of particle shape in the stress space [51]. An attempt has been made in this section to understand the relationship between the critical state and shape parameters. In Fig. 8a, the relationship between M and A_R is plotted. There is a strong linear relationship between these two quantities ($R^2 = 0.974$), indicating that the M values decrease with increasing A_R . A

strong correlation between M and C_X (Fig. 8b) and between M and S_W (Fig. 8c) both shows approximately linear relationships with acceptable regression coefficients values. These trends are in agreement with the study conducted by [51], for Fujian sand and Glass beads. Furthermore, considering the impacts of these three shape parameters (i.e. A_R , C_X , and S_W), the O_R as a shape index, the correlation between M and O_R is given as:

$$M = 2.197 - 1.384 O_R \quad (14)$$

The correlations between the critical state parameters (i.e. e_Γ and λ_c) and the shape parameters (i.e. A_R , C_X , S_W and O_R) are established in Fig. 9. It is seen that the e_Γ correlate with these shape parameters fairly well, giving linear relationships with acceptable regression values. Among the shape parameters, C_X correlate well with e_Γ (i.e. $R^2 = 0.981$). The shape effect on the intercept e_Γ can be well represented by O_R , is given as:

$$e_\Gamma = 1.435 - 0.747 (O_R) \quad (15)$$

The gradient of the CSL against the shape parameters is shown in Fig. 10. A fair correlation is established between λ_c and shape parameters. The CSL gradient decreases with

Fig. 8 Relationships between M and shape parameters

all three shape parameters. These findings are in agreement with those in the literature (e.g. [51]). Likewise, the effect of the shape parameter λ_c can be well represented by O_R , is given as:

$$\lambda_c = 0.0946 - 0.0862(O_R) \quad (16)$$

The above equation predicts that the slope of the CSLs in stress space tends to decrease as particle O_R increases. These findings are in agreement with the study conducted by [51].

5 Summary and conclusions

In this paper, a series of DEM based drained triaxial simulations are performed considering different values of η . The ultimate aim is to establish the relationships between critical state properties and shape parameters for the basic understanding of the mechanics of granular materials. Based on the analysis of results and discussions, the following findings can be drawn:

- The macroscopic response of granular materials exhibits post-peak strain-softening behaviour, and the stress ratio flattens off and tends to follow a steady-state after an axial strain of $\sim 40\%$. In addition, the residual shear strength of the assemblies depends on the applied confining stress.

Fig. 9 Relationships between e_T and shape parameters

- The critical strength of granular materials is found to be independent of the applied pressure and mainly influenced by the elongation parameter.
- The microscopic behaviour of granular materials in terms of CN shows an exponential decay against the axial strain. The deviator fabric follows a similar trend to the macro-scale behaviour of granular materials.
- Quantitative relationships have been established between the critical state and shape parameters using particles with different elongations. It should be highlighted that a critical stress ratio (M) and critical state parameters (i.e. e_T and λ_c) decrease with increasing shape parameter values in terms of aspect ratio, convexity, sphericity and overall regularity.

Fig. 10 Relationships between λ_c and shape parameters

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Compliance with ethical standards

Conflict of interest On behalf of all authors, the corresponding author states that there is no conflict of interest.

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