DEM7

The 7th International Conference on Discrete Element Methods
August 1 to August 4, 2016
Dalian, China

The Influence of Particles' Aspect Ratio on the Shear Behaviour of Granular Materials

Y.H. Xie[1], Z.X. Yang[1], D. Barreto[2]

Abstract: The mechanical response of granular material depends both on the material properties (e.g. stiffness, anisotropy, permeability, etc) and particle geometry (shape, roughness, etc.). This paper presents a study of the effect of particle shape (i.e. aspect ratio) on the mechanical behaviour of a granular assembly using DEM (discrete element method). In this study, the numerical simulations employ samples with different particle aspect ratios but identical particle size distribution (PSD). Conventional triaxial compression DEM simulations are carried out under both 'drained' and 'undrained' (constant volume) conditions. The shear behaviour of the assemblies and the evolution of the microstructure of the sample under shearing are examined in detail. At the macroscopic level, the test results show that the particle aspect ratio has a significant effect on the stress-strain curve, peak strength, dilatancy characteristics and critical state behaviour. In particular, the samples with lower aspect ratios can lead to higher peak/residual shear strengths, and higher angles of shearing resistance. The critical state occurs at a higher position in a void ratio versus mean normal stress plot for lowest particle aspect ratio. The results from numerical analysis compare reasonably well with the available experimental data. At the microscopic level, the fabric evolution is greatly affected by the aspect ratio.

Keywords: particle shape, granular material, discrete element method, shear behaviour, critical state, fabric evolution

1 Introduction

Granular materials are commonly encountered in nature and industry. For example, they are found in landslides and avalanches, raw minerals for extraction and transport, cereal storage, powder mixing, without forgetting cohesive frictional materials like concrete which are also made of granulates. The mechanical response of the granular materials is very complex and can be affected by many factors, including confining pressure, density, particle shape, particle size distribution loading path, etc.[1] It is recognised that particle characteristics affect the behaviour of granular soils. Recently, abundant experiment work has been undertaken to investigate the influence of particle characteristics on the mechanical response of granular materials. For example, Yang and Luo [2] employed spherical glass beads and crushed angular beads of mixtures with a uniform quartz sand to explore the relationship between the critical state behaviour and particle shape. Their experiments show that critical state behaviour and liquefaction potentials appear to be sensitive to the variation of shape parameters.

Over the years, DEM has demonstrated to be a powerful tool to improve the understanding of the fundamental behaviour of granular material. It cannot only capture the macro mechanical behaviour of the granular assembly but

[1] Y.H. Xie (✉)•Z.X. Yang
Department of Civil Engineering, Zhejiang University, Hangzhou, Zhejiang, China
e-mail: xieyh@zju.edu.cn

[2] D. Barreto
School of Engineering and the Built Environment, Edinburgh Napier University, Merchiston Campus, Edinburgh, EH10 5DT, Scotland

also the micro-scale variations simultaneously. A key feature of discrete element modelling is that the particles themselves are idealized entities with spherical elements being the most common type of particles considered in 3D DEM simulations. In the last several decades, many DEM based numerical simulations were performed to investigate the effect of particle shape on the mechanical behaviour of granular media. For instance, Nouguier [3] performed 2D numerical simulations with samples made of irregular hexagons with different particle elongation (i.e. ratio of maximum to minimum length)and found that the angle of shearing resistance decreases when the particle elongation increases for samples with equal initial density. Zhao et al [4] used a composite (clumped) particle model for non-spherical particles in DEM simulation and demonstrated that particle shape increases resistance to compaction. Anitha and Sitharam [5] studied the effect of particle aspect ratio on the monotonic shear behavior, however their study is limited to only two aspect ratios. Furthermore, a limited number of 3D DEM studies on the relationship of particle shape with critical state behaviour has been reported.

This study presents a comprehensive DEM analysis of particle aspect ratio effects on the mechanical behavior, including the shear strength, dilatancy characteristics, critical state responses, etc. A series of 'drained' and 'undrained' numerical experiments are performed with the specimens with varying aspect ratio, and a unique given particle size distribution. In addition, the micro-scale variations are also presented in terms of the fabric evolution, especially the quantification of the fabric at the critical state.

2 DEM Model and Particle Characteristic

2.1 DEM Model

The DEM method developed by Cundall and Strack [6] accounts for the particulate nature of soil and is capable of simulating both the macro- and micro-mechanical behaviour of granular material. In this paper, the open source DEM code originally developed by Kozicki and Donzé[7] is used. The DEM algorithm uses a time-centred finite difference scheme to find particle displacements from particle accelerations which in turn are found from the successive application of Newton's second law of motion and simple contact laws for the calculation of inter-particle forces.

2.2 Particle Characteristics

In general, particle shape is often characterized by elongation, roundness, angularity, texture etc [8]. The particle elongation is defined as illustrated in Fig. 1, by the ratio b/a (e.g. aspect ratio AR), where b is the length of the minor axis and a is the length of the major axis [9]. For a spherical particle AR=1, the higher the particle elongation the smaller the ratio AR. For the numerical DEM samples used in this study, the particle size distributions were chosen to replicate real sands. The size of the spherical particles considered in this study have a particle size range between 0.2-0.6mm in diameter. To vary the aspect ratio of the particles, clumped particles with desired ARs were created. Individual particle clumps have the same volume as the spherical particles. As a result, the samples composed of particles with different particle shape (aspect ratio) still have the same grading, as shown in Fig. 2. Table 1 shows the six different values of the particle aspect ratio AR considered in this study.

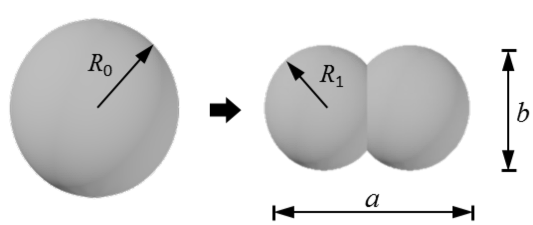


Fig. 1 Definition of particle aspect ratio AR

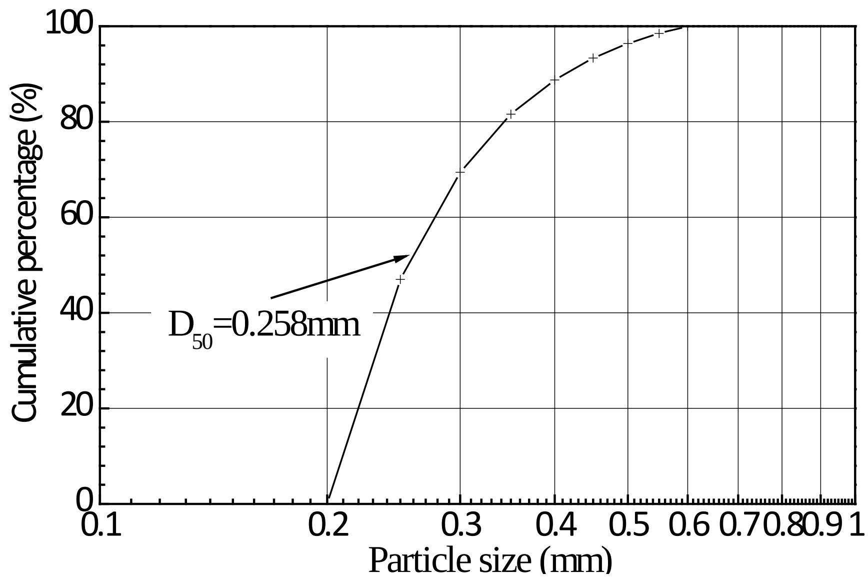
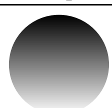
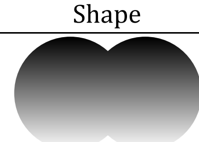
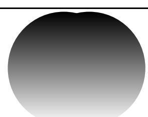
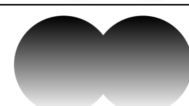
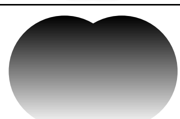
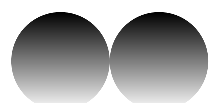


Fig. 2. Particle size distribution of assemblages employed in this study

Table 1 Particle aspect ratio AR

Shape	AR	Equivalent radius R	Shape	AR	Equivalent radius R
	1	r		0.625	1.215r
	0.833	1.09r		0.555	1.248r
	0.714	1.162r		0.5	1.26r

3 Numerical samples

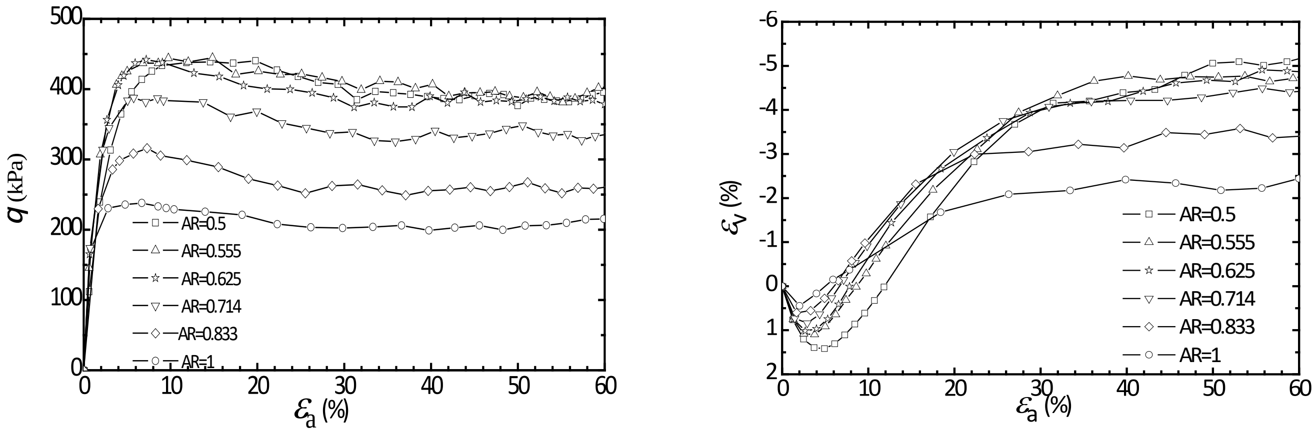
A cubic assemblage of particles with periodic boundaries is adopted in the simulation and enables to assess granular material behaviour free from boundary effects. After the desired number of clumped particles has been generated in a prescribed domain, the assemblage is then isotropically consolidated to a mean effective stress p'=200 kPa. Two staged consolidation is carried in this study. In the first stage, to obtain varying densities of the samples, different inter-particle friction coefficients are assigned onto the particles and the confining pressure is gradually increased to 180 kPa using a servo-control algorithm. In the second stage, the inter-particle friction coefficient is restored with a default value of 0.5 and the confining pressure is then increased to 200 kPa. After this, triaxial compressive shear under both 'drained' and 'undrained' conditions is performed under strain-control. Care was taken to ensure the simulations were quasi-static. During isotropic compression we used a strict criteria as unbalanced force ratio (<0.001) and as in other studies (i.e. [11]) we confirmed quasi-staticity during shear by performing a preliminary parametric study using different strain rates. A strain rate of 0.05 Hz was used in this study. To quantify the relative density RD of the samples, the maximum and minimal void ratios were determined from the reference state p'=10 kPa [12]. The parameters used in the simulations are summarized in Table 2.

Table 2 DEM Parameters used in the simulations

Sample ID	AR=0.5	AR=0.555	AR=0.625	AR=0.714	AR=0.833	AR=1

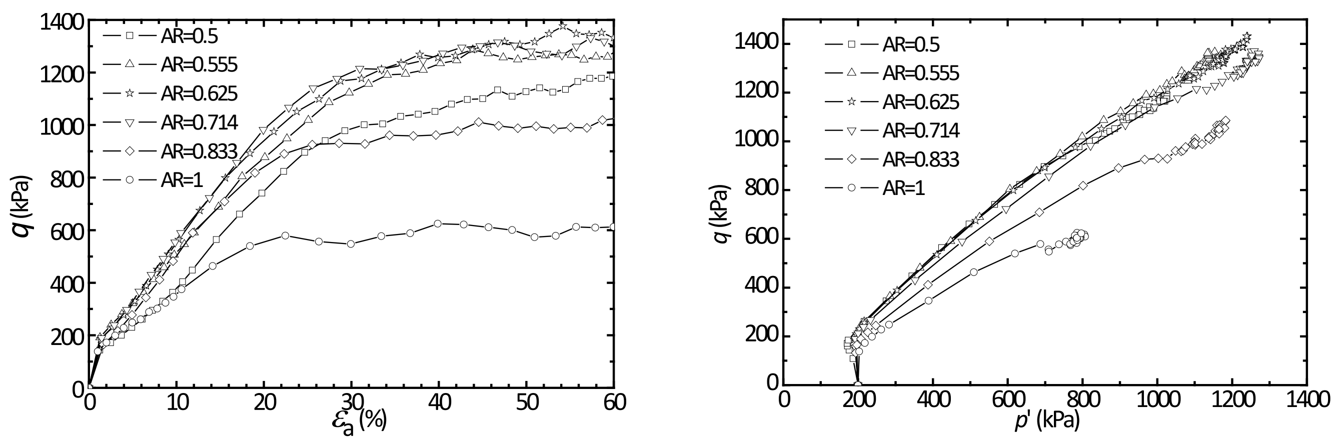
Particle density (10^6 kg/m^3)	2.65	2.65	2.65	2.65	2.65	2.65
Normal stiffness K_n/d (MPa)	100	100	100	100	100	100
Tangential stiffness K_s/d (MPa)	100	100	100	100	100	100
Relative density D_r (%)	20.5	20.1	20.3	20.4	20.2	20.8
Damping ratio	0.001	0.001	0.001	0.001	0.001	0.001
Unbalanced force ratio	0.001	0.001	0.001	0.001	0.001	0.001
Number of clumps N	10000	10000	10000	10000	10000	10000
Initial confining pressure p'_0 (kPa)	200	200	200	200	200	200
Strain rate (Hz)	0.05	0.05	0.05	0.05	0.05	0.05
Aspect ratio AR	0.5	0.555	0.625	0.714	0.833	1

4 Overall macroscopic behaviour



(a) (b)

Fig. 3. Drained responses of samples with varying ARs (p'_0=200 kPa, D_r=20%): (a) Deviatoric stress vs. axial strain; (b) volumetric strain vs. axial strain



(a) (b)

Fig. 4. Undrained responses of samples with varying ARs (p'_0=200 kPa, D_r=20%) :(a) Deviatoric stress vs. axial strain; (b) Effective stress paths

Fig 3 shows the drained triaxial test results of samples with p'_0=200 kPa and D_r=20% but with different particle aspect ratios. As can be seen in Fig. 3a, the deviatoric stresses increase to the peak values and then undergo softening behaviours, stabilizing at deviatroic strain ε_a=40% (approx.), which could be regarded as the critical state, as confirmed by examining the volumetric responses in Fig. 3b. In general, the critical deviatoric stress falls with the AR. The spherical particles (AR=1) have the minimum value. It is also found that then when AR > 0.625, there is no significant difference in both the stress-strain and volumetric responses. As observed in Fig. 3b, all the samples experience an initial contraction followed by dilation. It is also clear that as the aspect ratio increases, the dilatancy reduces. This suggests the particle aspect ratio considerably affects the dilatancy response for the granular soils. This can be intuitively justified by the inhibited particle rotation experienced by non-spherical particles (i.e. AR ≠ 1) during shearing.

Figure 4 presents undrained triaxial test results of samples with p'_0=200 kPa and D_r=20% but with different particle aspect ratios. As shown in Fig. 4a, the deviatoric stresses at large strain level ε_a>=40% are flattened off and tend to reach constant values at critical state, which depend on the aspect ratio AR of the samples. Fig. 4b shows the effective stress paths, indicating that all the samples experience "contractive" behaviour prior to the "dilatant" behaviour with higher effective stresses towards to the critical state.

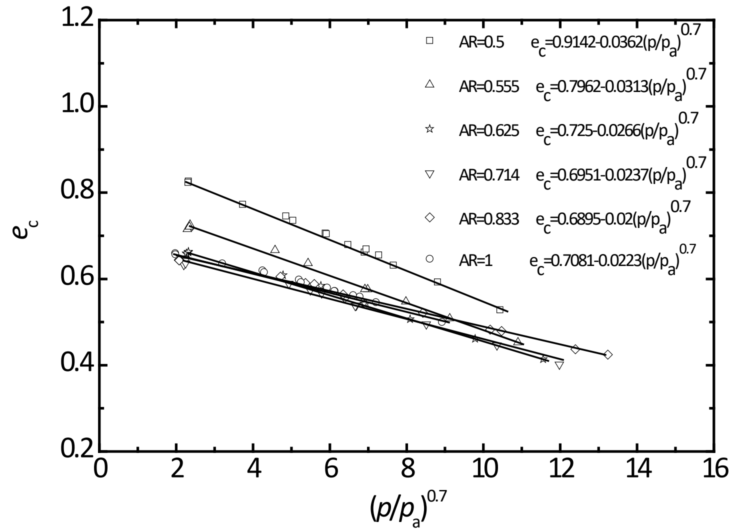


Fig. 5. Critical state line at $e-p'$ plane

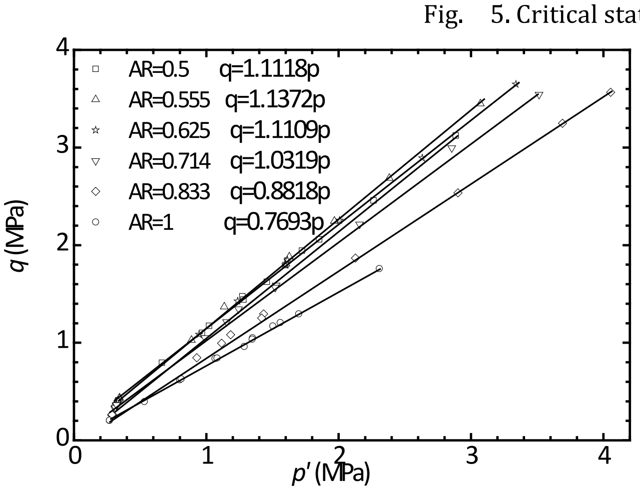


Fig. 6. Critical state line $p'-q$ plane

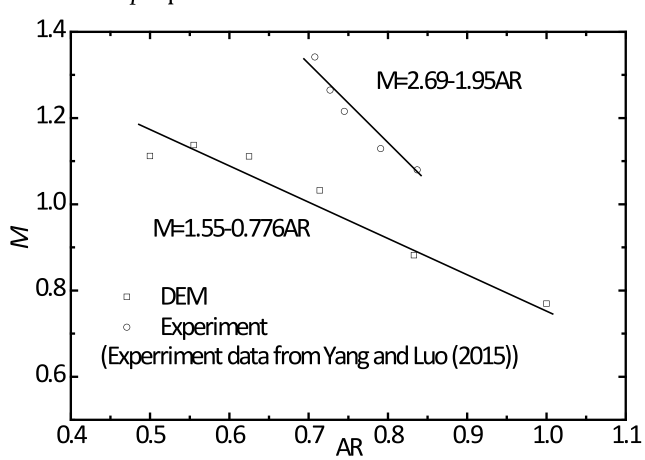


Fig. 7. Critical stress ratio vs particle aspect ratio

To explore the relationship between critical state and particle aspect ratio, additional numerical tests for each aspect ratio were conducted, with varying conditions such as density, confining pressure, and drainage conditions. Critical state is defined as the state only deforming in shear without change in stresses and volume [13], i.e.

$$\dot{p}=0, \quad \dot{\mathbf{s}}=\mathbf{0}, \quad \varepsilon_v=0 \quad \text{But} \quad \dot{\mathbf{e}}=\mathbf{0} \tag{1}$$

where p is the mean normal effective stress, $\mathbf{s}$ the deviatoric stress tensor, ε_v the volumetric strain, $\mathbf{e}$ the deviatoric strain tensor, and a superposed dot denotes the rate. Upon reaching the critical state, the stress ratio $\eta=q/p$ and the void ratio e will satisfy the following conditions,

$$\eta=\eta_c=(q/p)_c=M \quad \text{and} \quad e=e_c=\hat{e}(p) \tag{2}$$

And Li [14] proposed a linearization approach to straighten the critical state line (CSL) in the $e\text{-}\left(p'/p_a\right)^{\xi}$ plane, which can be expressed into,

$$e_c = e_\Gamma - \lambda_c \left(p'/ p_a \right)^{\xi} \tag{3}$$

in which p_a is the atmospheric pressure serving as a reference pressure for normalization, e_Γ is the intersection of CSL on e-axis at $p'=0$, λ_c is the slope of the line and ξ is a parameter used for fine tuning for optimization. It is seen that to determine the CSL, three material constants are required. However, the straightness of the CSL is insensitive to the parameter ξ, which can be assumed to be 0.7 for simplicity.

5 Microscopic observations

It is noted that unlike the conventional physical tests, DEM simulations can provide more insights into the microscopic responses of the granular assemblages. The term 'fabric' is frequently used to represent the microstructure of the granular materials, which may be subject to variations during shear. We will examine herein how the fabric evolves towards the critical state for samples with different aspect ratios, in order to understand the underlying mechanism associated with distinct macroscopic behaviours outlined above. From a microstructural perspective, for an aggregate having N measurements of the quantities that reflect the microstructures of the granular media, such as particle orientation, contact vector normal, branch vector etc., the fabric can generally be represented by the deviatoric part **F** of a tensor **G** according to

$$\mathbf{F} = \frac{\mathbf{G}}{tr\left(\mathbf{G}\right)/3} - \mathbf{1} \quad \text{with} \quad \mathbf{G} = \frac{1}{2N}\sum_{k=1}^{2N} w(\mathbf{m}^k)\mathbf{m}^k \otimes \mathbf{m}^k \tag{4}$$

where $\mathbf{m}^k$ is a unit vector along the k-th measurement of the characteristic direction, say, the direction of contact normal [16], and the $w(\mathbf{m}^k)$ is a weighting factor. If $w(\mathbf{m}^k)$=1 as in the case of contact normal based definition, tr **G** =1, a trivial constant. Henceforth the **F** will be called the fabric tensor in the entire paper. In order to identify the norm F and direction $\mathbf{n}_F$ of **F** one can write

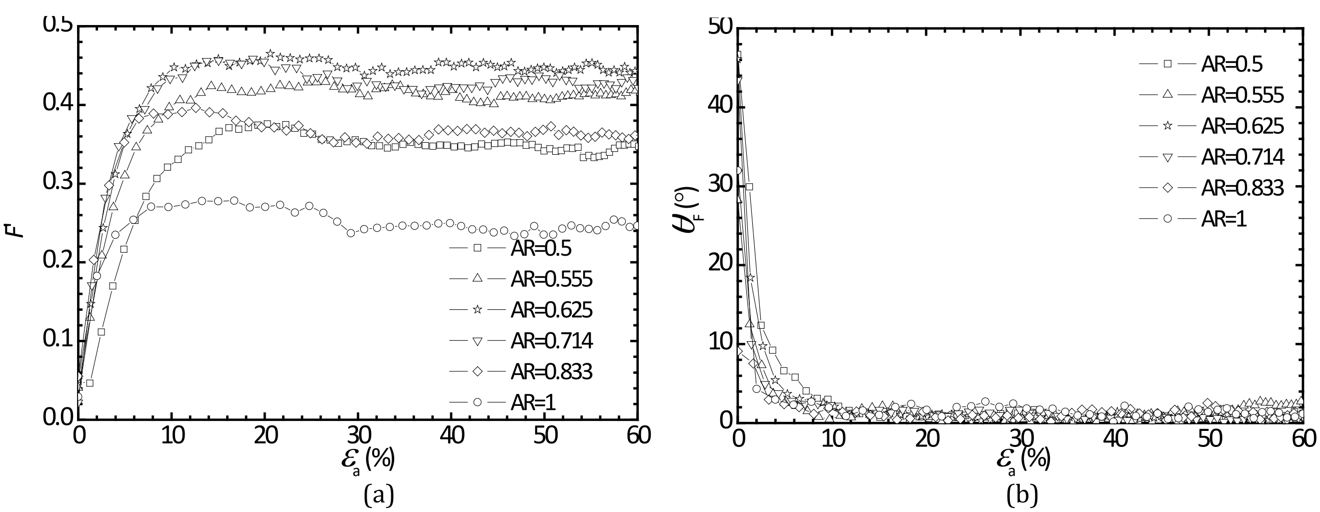
$$\mathbf{F} = F\mathbf{n}_F, F = \sqrt{\mathbf{F}:\mathbf{F}}, \mathbf{n}_F : \mathbf{n}_F = 1, tr\mathbf{n}_F = 0 \tag{5}$$

Clearly, **F** possesses two none-trivial invariants: the norm F and the lode angle θ_F associated with $\mathbf{n}_F$ by expression $\cos 3\theta_F = \sqrt{6} tr\mathbf{n}_F^3$, in which $0^\circ \le \theta_F \le 60^\circ$, with $\theta_F = 0^\circ$ for triaxial compression while $\theta_F = 60^\circ$ for triaxial extension.

To restore the density measure of the fabric tensor, the easiest approach is to normalize the **F** with the specified function of void ratio e, which can be tentatively expressed into.

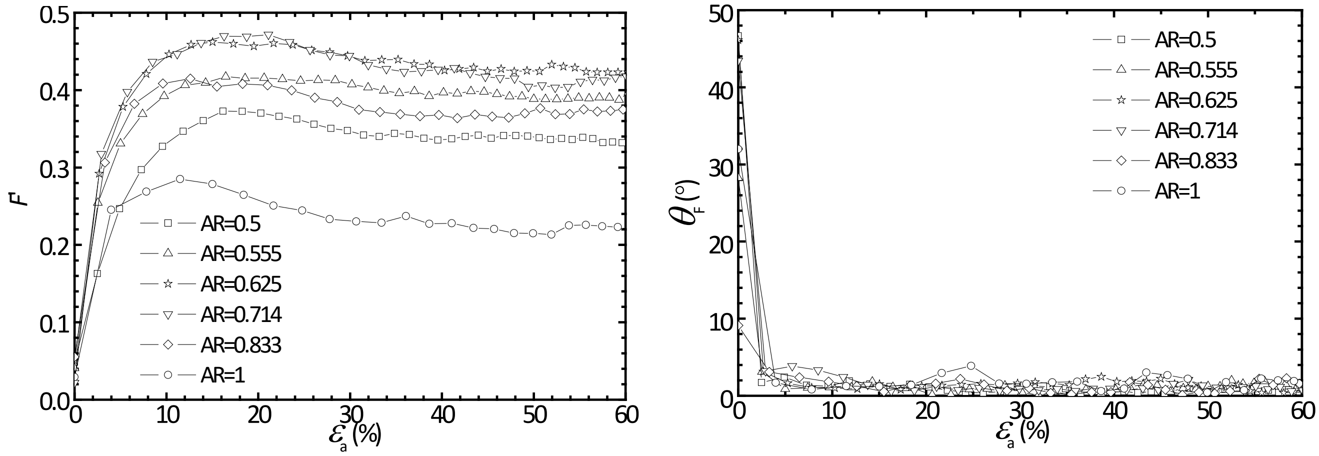
$$\mathbf{F}' = \mathbf{F}/\left(1 + e + e^2\right) \tag{6}$$

According to ACST [17], the normalize fabric norm attain a unique value for triaxial compression test. That is to say, it is independent of critical void ratio and critical mean effective stress.



(a) (b)

Fig. 8. Fabric evolution for drained simulations (p'_0=200 kPa, D_r=20%) :(a) Normalised fabric norm vs. axial strain; (b) Lode angle vs. axial strain

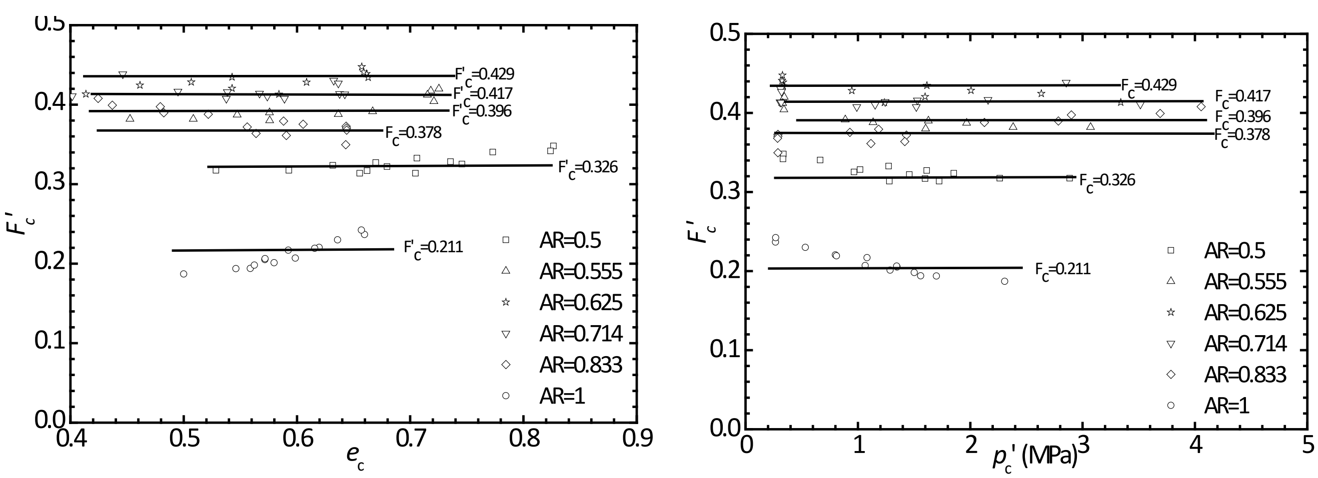


(a) (b)

Fig. 9. Fabric evolution for undrained simulations: (p'_0=200 kPa, D_r=20%) :(a) Normalised fabric norm vs. axial strain; (b) Lode angle vs. axial strain

Shown in Fig. 8 is the evolution of fabric for drained simulations. Fig. 8a presents the evolution of the norm F of the fabric tensor, which increases with the deviatoric strain but tends to be flattened off when reaching constant values at critical state (ε_a>=40%) It is noted that the critical norm of the sample with AR=0.625 is the greatest while it is smallest for sample composed of spherical particles (AR=1). Fig. 8b illustrates the Lode angle θ_F evolutions against the deviatroic strains. It is seen that unlike the fabric norm, θ_F decreases with the strain and stabilizes at 0 around ε_a=40%, indicating that the fabric direction is co-directional with the loading direction at the critical state. Similar observations can also be found from undrained simulations, as illustrated in Fig. 9.

The fabric evolution can also be stable in critical state and it can be added to the critical state. Fig. 10a presents the critical fabric norm against the critical void ratio. There is some scatter in the data, but a trend can be observed for each particle aspect ratio achieving a constant value. It means that the critical fabric norm is independent of critical void ratio. As shown in Fig 10b, the critical fabric norm is also independent of critical mean effective stress.



(a) (b)

Fig. 10. Normalised critical fabric norm: (a) Critical void ratio; (b) Critical mean effective stress

7 Conclusions

This paper presents a systematic DEM analysis of the effect of particle aspect ratio effects on the mechanical behaviour of granular materials. It has shown that the aspect ratio of the particles in the assemblages have a significant influence on the shear strength, dilatancy and critical state behaviour. The microscopic responses are also examined in terms of the fabric evolutions during shear. The main observations can be summarized as follows:

1. The DEM can simulate different particle aspect ratios to account for particle shape effects, while also considering different initial densities. Furthermore, a critical state and fabric evolution can be attained.
2. Both undrained and drained tests provide evidence that particle aspect ratio can significantly alter the stress-strain behaviour of granular materials.
3. The critical fabric norm is independent of critical void ratio and critical mean effective stress. An increasing particle aspect ratio causes a change in the value of the critical fabric norm.
4. It has been established that the particle aspect ratio can influence the critical state properties. However, it has been demonstrated that this effects "saturates" as AR increases. For AR >0.625, critical state line in $p-q$ plane appear to be insensitive to further increase on the particle aspect ratio.

Acknowledgement

The research described was funded by the National Key Basic Research Program of China (No.2015CB057800) and Natural Science Foundation of China (Nos. 51578499 & 51322809). Their support is gratefully acknowledged.

References:

[1]. CAVARRETTA, I., M. COOP and C. O'SULLIVAN, The influence of particle characteristics on the behaviour of coarse grained soils. Géotechnique, 2010. 60(6): p. 413-423.
[2]. Yang, J. and X.D. Luo, Exploring the relationship between critical state and particle shape for granular materials. Journal of the Mechanics and Physics of Solids, 2015. 84: p. 196-213.
[3]. Nouguier-Lehon, C., B. Cambou and E. Vincens, Influence of particle shape and angularity on the behaviour of granular materials: a numerical analysis. International Journal for Numerical and Analytical Methods in Geomechanics, 2003. 27(14): p. 1207-1226.
[4]. Zhao, T., et al., A composite particle model for non-spherical particles in DEM simulations. Granular Matter, 2015. 17(6): p. 763-774.
[5]. Anitha Kumari, S.D. and T.G. Sitharam, Effect of Aspect Ratio on the Monotonic Shear Behaviour: Micromechanical Interpretations. Geotechnical and Geological Engineering, 2013. 31(5): p. 1543-1553.
[6]. Cundall, P.A. and O.D. Strack, A discrete numerical model for granular assemblies. Géotechnique, 1979. 1(29): p. 47-65.
[7]. Kozicki, J. and F.V. Donzé, A new open-source software developed for numerical simulations using discrete modeling methods. Computer Methods in Applied Mechanics and Engineering, 2008. 197(49-50): p. 4429-4443.
[8]. Cho G C, D.J.S.J., Particle Shape Effects on Packing Density, Stiffness, and Strength: Natural and Crushed Sands. Journal of Geotechnical and Geoenvironmental Engineering, 2006. 5(132): p. 591-602.
[9]. Yang, Z.X., J. Yang and L.Z. Wang, On the influence of inter-particle friction and dilatancy in granular materials: a numerical analysis. Granular Matter, 2012. 14(3): p. 433-447.
[10]. Guo, N. and J. Zhao, The signature of shear-induced anisotropy in granular media. Computers and Geotechnics, 2013. 47: p. 1-15.
[11]. Kuhn M R, R.H.E.M., Investigation of Cyclic Liquefaction with Discrete Element Simulations. Journal of Geotechnical and Geoenvironmental Engineering, 2014. 140(12).
[12]. Salot, C., P. Gotteland and P. Villard, Influence of relative density on granular materials behavior: DEM simulations of triaxial tests. Granular Matter, 2009. 11(4): p. 221-236.
[13]. Yang, Z.X., J. Yang and L.Z. Wang, Micro-scale modeling of anisotropy effects on undrained behavior of granular soils. Granular Matter, 2013. 15(5): p. 557-572.
[14]. Li X S, W.Y., LINEAR REPRESENTATION OF STEADY-STATE LINE FOR SAND. Journal of geotechnical and geoenvironmental engineering, 1998. 124(12): p. 1215-1217.
[15]. Yan, W.M., Fabric evolution in a numerical direct shear test. Computers and Geotechnics, 2009. 36(4): p. 597-603.
[16]. Oda, M.K.J.A., Experimental micromechanical evalutation of strength of granular materials: effects of particle Experimental micromechanical evalutation of strength of granular materials: effects of particle rolling. Mechanics of materials, 1982. 1(4): p. 269-283.
[17]. Li, X.S.A.D., Anisotropic Critical State Theory: Role of Fabric. Journal of Engineering Mechanics, 2012. 3(138): p. 263-275.