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Analysis of granular assembly deformation using discrete element method

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Abstract: The discrete element method is used to simulate specimens under three different loading conditions (conventional triaxial compression, plane strain, and direct shear) with different initial conditions to explore the underlying mechanics of the specimen deformation from a microscale perspective. Deformations of specimens with different initial void ratios at different confining stresses under different loading conditions are studied. Results show that the discrete element models successfully capture the specimen deformation and the strain localization. Particle behaviors including particle rotation and displacement and the mesoscale void ratio distributions are used to explain the strain localization and specimen deformation. It is found that the loading condition is one of the most important factors controlling the specimen deformation mode. Microscale behavior of the granular soil is the driving mechanics of the macroscale deformation of the granular assembly.

Key words: granular soil; loading condition; deformation mode; numerical simulation; strain localization

The soil failure deformation mode is an important issue in geotechnical engineering that relates to both the strength and the functionality of geotechnical structures. Conventional triaxial compression (CTC), plane strain (PS), and direct shear (DS) are the three mostly used laboratory tests to simulate the field conditions. Soils subjected to different loading conditions show different failure deformation modes. Deformation modes of specimens under different loading conditions have been extensively studied[1]. However, there are still some contradictory results from different researchers using different methods. What is more, the driving micromechanics that govern deformation behaviors, particularly in soils that fail via regions of high localized strain (e. g., shear banding), are still unclear. The discrete element method (DEM) has gained increasing popularity over recent years and it is considered to be a powerful tool for simulating granular materials, especially from the viewpoint of microscale and micromechanics[2].

In this paper, the deformation mode of a granular material is numerically investigated under three different loading conditions, PS, CTC, and DS. Numerical experiments are performed using the commercially available three-dimensional discrete element method code PFC^{3D}. Particle behaviors including particle rotation and particle displacement and the mesoscale void ratio are used to explain the specimen failure deformation from the perspective of microscale.

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1 Numerical Model

The discrete element model is composed of distinct particles which displace independently and interact only through contacts or interfaces between the adjacent particles. Walls are used to simulate the boundary conditions. Newton's second law and the force-displacement law are the two basic theories and calculations. Different contact constitutive models including the stiffness model, the slip model, the bonding model and some alternative models can be used to simulate different situations. More details about the DEM can be found in Ref. [3].

Every effort has been made to select model parameters that are consistent with physical counterparts from a uniformly graded clean quartz sand (e. g., Ottawa 20-30 sand). Each particle is comprised of two identical overlapping spheres (radius ranges from 0. 10 to 0. 15) clumped together so that the aspect ratio (length/width) is 1. 5 : 1, which can avoid a significant overestimation of particle rotations of spherical particles during shear[4]. Right orthorhombic specimens with a 7 : 4 : 2 ratio for PS, right cylinders with a 2 : 1 ratio for CTC, and square horizontal cross-section with a 1 : 1. 5 ratio for DS model dimensions are used, which are consistent with standard laboratory practices. Additional material properties are shown in Tab. 1.

Tab. 1 Some material properties for numerical simulations

Normal stiffness/ (N · m^{-1})	Shear stiffness/ (N · m^{-1})	Friction coefficient	Specific gravity	Platen friction coefficient
10^8	10^7	0. 31	2. 65	0

Accurate modeling of membrane confinement is especially critical for study of the deformation of the specimen from both macro- and micro-scale. In this study, a new method of using stacks of planar (for PS and DS tests) or cylindrical walls (for the CTC test) to simulate the membrane is proposed. This method is proved to be more accurate, more efficient, and easier than the previous methods such as rigid wall[5], periodic boundary[6], and flexible wall[7]. Mass scaling, which is commonly used by many researchers[8], is employed in the simulations to decrease computation time.

Two factors that have significant effects on the failure deformation mode of the sample, the initial void ratio and the confining stress, are considered here. Simulations are performed on loose (e_0 = 0. 67) and dense (e_0 = 0. 47) specimens at low (σ_3' = 75 kPa) and high (σ_3' = 450 kPa) confining stresses.

Deviatoric stress (PS and CTC) or stress ratio (DS) and volumetric strain as a function of global axial strain (ε_1) for each simulation are presented in Figs. 1 (a), (b), and (c)

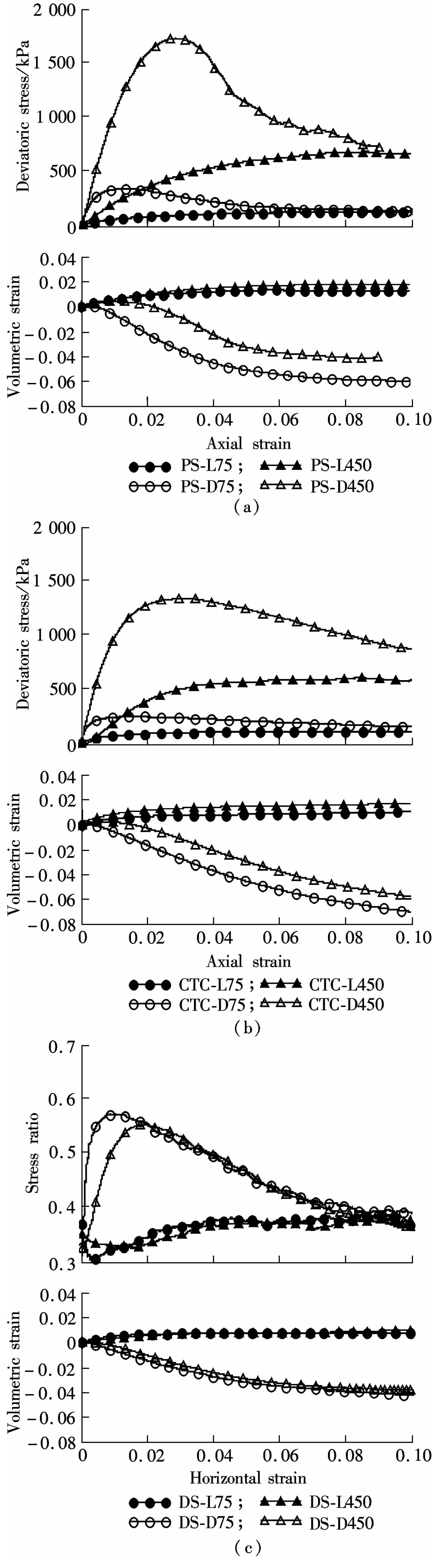

Fig. 1 Deviatoric stress (stress ratio) and volumetric strain vs. axial strain. (a) PS; (b) CTC; (c) DS

for PS, CTC, and DS, respectively. PS-L75, for example, means the loose plane strain specimen at a confining stress of 75 kPa. It can be seen from Fig. 1 that denser specimens show peak deviatoric stresses or peak stress ratios and dilatant behavior, while looser specimens contract and do not exhibit peak deviatoric stress. At the same time, a lower void ratio and a higher confining stress result in higher peak strengths. These results are consistent with those obtained from laboratory experiments[1]. This indicates that the current models are capable of reproducing the macroscale material response of granular assemblies in a manner consistent with that observed in physical experiments and consequently capable of capturing the characteristics of assembly deformation. These figures further illustrate that the medium and dense CTC specimens have likely not yet reached critical states at the maximum axial strain considered in the simulations (10%), although they generally appear to be trending toward constant stress and volume. This may indicate that the CTC specimen needs larger strain to reach a critical state.

2 Failure Deformation

Samples under different loading conditions have different failure deformation shapes. These differences are related to the failure mechanics and the specimen microstructure at the failure state. Abundant research on failure deformation of specimens under different boundary conditions has been performed. Strain localization or shear banding is a well observed phenomenon in many laboratory experiments. The region of strain localization is considered to have a governing role in the strength response and the volumetric behavior of the specimen.

Final deformation shapes of all the specimens (dense and loose specimens at low (75 kPa) and high (450 kPa) confining stresses) can be seen from Fig. 2. For PS specimens, Fig. 2 (a) shows that the dense sample has two apparent shear bands at the low confining stress but only one at the high confining stress. The loose sample deforms more homogeneously and it becomes short with a little bit bulging without apparent shear band at both low and high confining stresses. For CTC specimens, Fig. 2 (b) indicates that all the specimens bulge more or less but do not show obvious shear band at the final state. With the same confining stress, the dense sample bulges more and the loose sample deforms in a more homogeneous manner than the dense sample and with more shortening than bulging. This is true for both high and low confining stresses. For DS specimens, since the shearing plane is specified by the device, the failure plane is subsequently given. There is no significant qualitative difference in the failure deformation shape for all the tests as shown in Fig. 2 (c).

These results indicate that the loading condition is the first factor governing the deformation mode of the specimen. With the same loading condition, both the density and the confining stress have influences on the strain localization in the sample, and density has more effects than confining stress. For CTC specimens, although there is no obvious shear band from the deformation shapes, it does not necessarily mean that no localization occurs in these specimens. Just as pointed out by Desrues et al. [9], the bulging is only an external manifestation and the internal failure pattern is more complex.

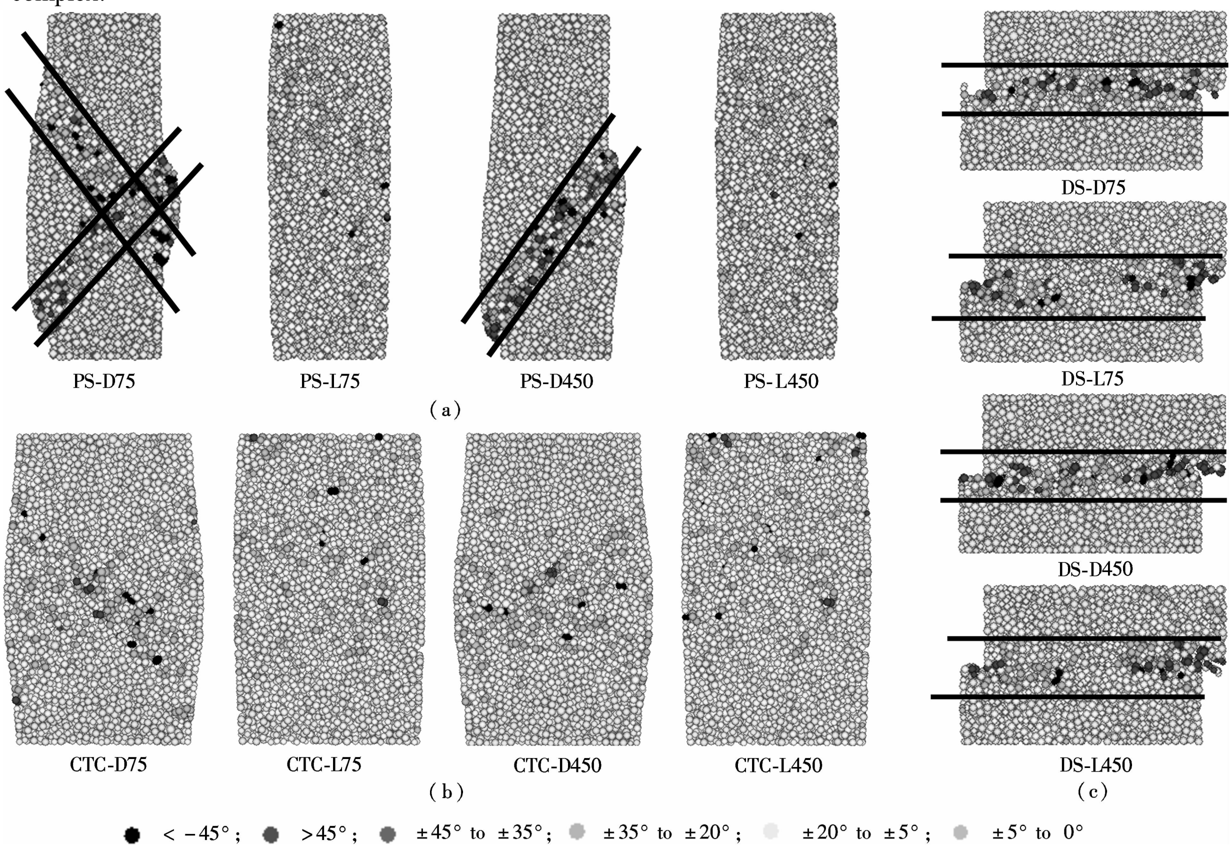

Fig. 2 Particle rotations. (a) PS simulation; (b) CTC simulation; (c) DS simulation

3 Microscale Analysis of Deformation Mode

Macroscale exhibition of the specimen deformation under different loading conditions is considered to be the consequence of the microscale particle behavior and the microstructure change of the specimen. Particle behaviors including particle rotation and particle displacement and microstructure property, the local void ratio, are used to explain the behavior of specimen deformation under different conditions.

3.1 Particle rotation

The particle rotation of the specimen subjected to loading is a well-recognized phenomenon. For example, Suiker and Fleck[10] mentioned that the prevention of particle rotations resulted in an increment of deviatoric strength by a factor of two to three from numerical study. Oda and Kazama[11] observed a sharp change of particle orientation at the boundaries of shear band, which indicates a high gradient of particle rotation in a narrow zone. These indicate that particle rotation has great effects on both strength and deformation of the granular soils.

As mentioned above, the clump particle which is comprised of two identical spheres that overlap with an aspect ratio of 1.5 is used to avoid the significant overestimation of particle rotations of spherical particles. Particle rotations of the specimens under different loading conditions are presented in Fig. 2. In these figures, different colors are used to indicate different magnitudes of particle rotations. For PS tests, in dense specimens, particle rotations have higher magnitudes in narrow zones which correspond to the strain localization called shear bands. Two shear bands can be identified by the particle rotations for the specimen at low confining stress but only one for the specimen at high confining stress, which shows the effect of confining stress on strain localization. In the loose specimens, particle rotation is more homogeneous with no localized concentration observed, which is quite different from the dense specimens.

For CTC tests, particle rotations have a higher magnitude in the middle of the specimen than near the platens in the dense specimens. But no obvious narrow band concentration of particle rotation is observed, which is different from PS specimens. Similar to PS simulations, particle rotations are more homogeneously distributed and there is no localized concentration in the loose specimens.

In the DS simulations (see Fig. 2(c)), particle rotations in the pre-defined shear plane are higher. For specimens with the same initial density, higher overburden stress corresponds to the narrower region of high particle rotations. These plots clearly indicate an inclined, rather than horizontal, plane of shear consistent with the kinematic constraints of the DS test.

3.2 Particle displacement

Particle motion can be decomposed into two parts, rotation and displacement. Particle displacement behaviors in discrete simulations have been previously investigated[12], but these studies have focused on a specific boundary condition. In this study, particle displacement behaviors are explored to explain the different deformation modes of the specimens under different loading conditions.

Particle displacement contour plots at terminal strain for

PS, CTC, and DS simulations are shown in Fig. 3, in which the absolute values of particle displacement are used. The results are very similar to those of particle rotations. In PS simulations, obvious bands are observed which indicate the localization of strain. Two well-defined shear bands are observed in the dense specimens at the low confining stress but only one at the high confining stress. Conversely, no distinct shear band is observed in the loose specimens. CTC simulations exhibit lower particle displacements in the middle of the specimen relative to the end platens. The loose specimens have more homogeneous particle displacements. In DS simulations, shear planes can be observed along the plane of predefined shear. Similar to PS tests, the dense specimens have more distinct shear bands than the loose specimens and the shear band thickness of the dense specimens is less than that of the loose specimens.

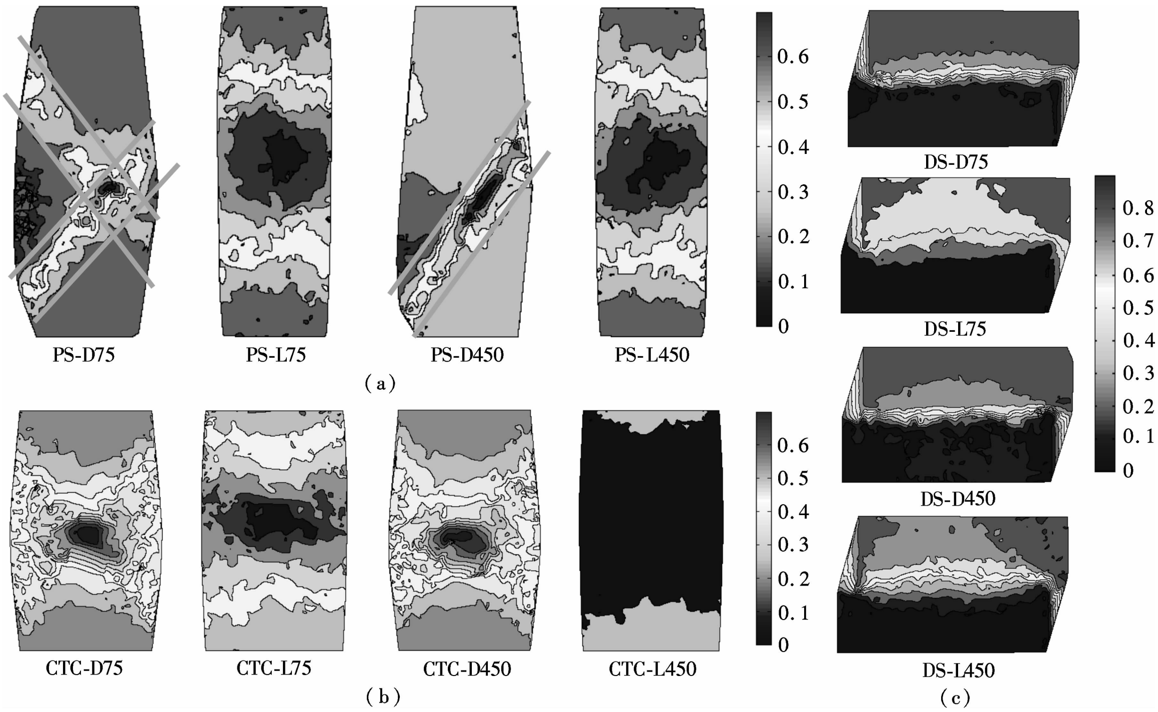

Fig. 3 Particle displacement contours. (a) PS simulation; (b) CTC simulation; (c) DS simulation

One important phenomenon observed from both particle rotation and displacement is the conical zone near the platens in the CTC dense specimens. In these zones, the particle rotations and displacements are small. This reflects the constraint role of the platens in the particle motion as well as in the specimen deformation. This phenomenon is consistent with the observation from previous laboratory experiments[13].

From the analyses of particle rotation and particle displacement, the specimen deformation modes under different loading conditions with different initial conditions are clearly exhibited. Strain localization is shown to be an important phenomenon of the granular soil. The particle behaviors inside and outside the strain location zone are quite different. It can be concluded that the microscale behaviors such as particle rotation and particle displacement are the underlying physics of macroscale deformation of the specimen.

3.3 Void ratio

Void ratio is one of the best recognized parameters that play a significant role in governing the strength of the soil. Void ratios inside and outside of the strain localization zone have been found to be different. It has also been proved to be an important indication of specimen deformation by some researchers from the results of both the experimental method[7] and the numerical method[14]. In this study, the void ratios within spheres at different positions are measured and the void ratio distributions within the specimen are obtained. Spherical measurement volumes with radii of two times the mean particle diameter are used with neighboring measurement volumes overlapping each other by one radius. A representative central plane within the specimen is used to present the void ratio distribution of the specimen.

Fig. 4 presents the void ratio contours on a central plane in the specimens. In PS simulations, two narrow bands with high void ratios are observed in the dense specimens at low confining stress but only one at high confining stress, indicating that higher confining stress tends to suppress the occurrence of strain localization. These narrow bands correspond to shear bands in the dense specimens. Void ratios are more homogeneously distributed in the loose specimens with no obvious occurrence of strain localization. In CTC simulations, for the dense specimens, the void ratios in the middle part of the specimens are higher than those at the upper and lower parts of the specimens, indicating diffuse failure, but no distinct shear plane is observed. The loose specimens have a more homogeneous void ratio distribution with no strain localization being observed. This corresponds to a shortened non-bulging deformation. In DS simulations, void ratios near the pre-defined shearing plane are greater than those away from the plane such that a band of high void ratios can be identified in all simulations.

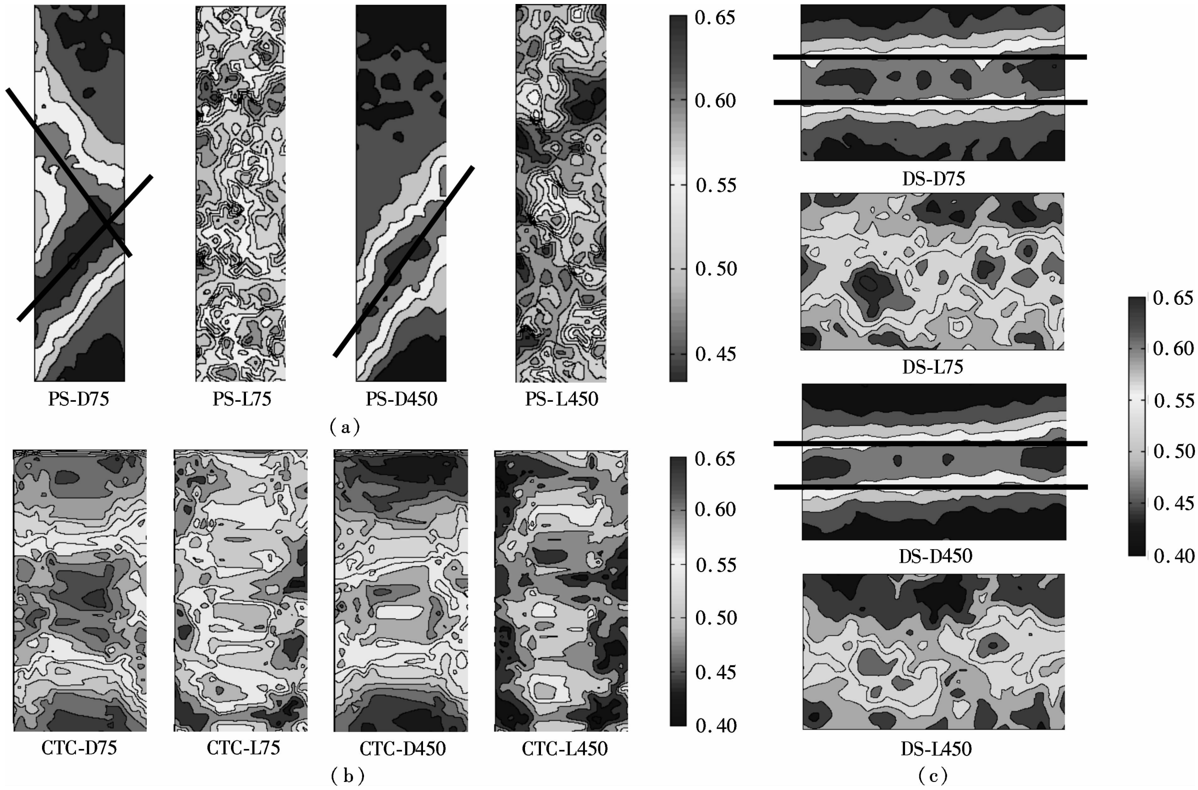

Fig. 4 Void ratio contours of assembly central plane. (a) PS simulation; (b) CTC simulation; (c) DS simulation

4 Strain Localization

Strain localization has a pronounced effect on the behavior of granular materials. The literature contains significant research pertaining to strain localization based on experimental and numerical work. In this study, strain localization is evident in the analyses of particle rotation, particle displacement, and void ratio distribution from the viewpoint of microscale.

Configurations, including inclination and thickness, of the shear band are of interest to many researchers and extensive work has been done using different methods. There are three most historically significant theoretical solutions for shear band inclinations, which were proposed by Coulomb[15], Roscoe[16], and Arthur et al[17]. They can be expressed as

$$\theta_C = 45° + \frac{\varphi_p}{2} \tag{1}$$

$$\theta_R = 45° + \frac{\psi_p}{2} \tag{2}$$

$$\theta_A = 45° + \frac{\varphi_p + \psi_p}{2} \tag{3}$$

where θ_C, θ_R, and θ_A are the shear band inclinations predicted by Coulomb, Roscoe, and Arthur et al., respectively; ϕ_p is the peak friction angle, and ψ_p is the peak dilatancy angle. In this study, shear band inclinations are the visually approximated in the dense PS specimens as shown in Figs. 2 to 4. The measured values as well as the calculated value from Eqs. (1) to (3) are presented in Tab. 2. Measured shear band inclinations in the numerical simulations are the closest to those predicted by Roscoe. It is likely that the current simulations result in these lower bound shear band inclinations because of the relative uniformity in particle size and shape relative to physical soils.

Tab. 2 Measured and predicted shear band inclination (°)

Simulations	Measured	Ref. [15]	Ref. [16]	Ref. [17]
PS-D75	55/47	68	57.6	62.8
PS-D450	54	66.6	55.5	61

Shear band thickness values reported in the literature are not in good agreement. The values vary from approximately 5 to 20 times the mean particle diameter with larger particle sizes correlating to thinner shear bands. Harris et al. [18] reported thicknesses typically 12 to 17 times the mean particle diameter based on PS experiments while Oda and Kazama[11] reported 7 to 8 times the mean particle size. Evans[7] reported 11 to 12 times d_{50} of the particle from experimental results and 15 to 19 times d_{50} from 2D numerical simulations. The thicknesses of the shear bands measured in this study are found to be approximately 7 times the mean particle size for PS specimens and 9 times for DS specimens. The results are close to the conclusion from Oda and Kazama[11].

5 Conclusion

A series of discrete numerical simulations is performed to explore the effects of loading conditions on specimen deformation of granular assemblies. Three loading conditions, CTC, PS, and DS, are studied for specimens with low and high initial void ratios at low and high confining stresses. Particle behaviors including particle rotation and particle displacement and the void ratio distributions are studied to reveal and explain the specimen deformation from a microscale perspective. Different strain localization modes under different conditions are clearly exhibited by these microscale parameters. The loading condition is found to be the first factor determining the failure deformation mode of the specimen. Density is shown to have more effects on the specimen deformation than the confining stress. Higher confining stress is found to tend to suppress the occurrence of strain localization. Strain localization configurations (inclination and thickness) of assembly under different loading conditions are investigated based on the study of particle rotation, particle displacement, and the mesoscale void ratio.

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颗粒集合体变形破坏特征离散元计算分析

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摘要:应用离散单元法研究了颗粒土试样在传统三轴压缩、平面应变和直剪 3 种不同荷载条件及不同初始条件下的变形破坏特性,从微观角度分析了不同条件下颗粒土试样变形的根本物理机理. 对不同初始孔隙比、不同围压、不同荷载条件下的试样变形和破坏进行了数值模拟计算分析. 结果表明,离散单元法可以准确反映试样的变形情况和局部应变等特性. 通过对微观颗粒行为包括颗粒旋转和颗粒平移及局部孔隙率的研究,从细微观角度解释了不同条件下试样的变形特性和局部应变的产生机理,结果显示,荷载条件是影响试样变形破坏模式的重要因素,土的微观行为特性是其宏观表现特性的根本的内在物理原因.

关键词:粒状土;荷载条件;变形模式;数值模拟;局部应变

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