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Discrete element modeling of sand behavior in a biaxial shear test*

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Abstract: The mechanical behavior of sand is very complex, and depends on factors including confining pressure, density, and drainage condition. A soil mass can be contractive or dilative when subjected to shear loading, and eventually reaches an ultimate state, referred to as the critical state in soil mechanics. Conventional approach to explore the mechanical behavior of sand mainly relies on the experimental tests in laboratory. This paper gives an alternative view to this subject using discrete element method (DEM), which has attracted much attention in recent years. The implementation of the DEM is carried out by a series of numerical tests on granular assemblies with varying initial densities and confining pressures, under different test configurations. The results demonstrate that such numerical simulations can produce correct responses of the sand behavior in general, including the critical state response, as compared to experimental observations. In addition, the DEM can further provide details of the microstructure evolutions during shearing processes, and the resulting induced anisotropy can be fully captured and quantified in the particle scale.

Key words: Granular soil behavior, Critical state, Microstructure, Discrete element method (DEM)
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INTRODUCTION

Granular soil behavior is of general interest in soil mechanics, and upon loading, sand contracts in its loose state, and dilates in its dense state. However, whether the sand in the loose or dense state is not merely determined by its density, but also due to the applied confining pressure (Verdugo and Ishihara, 1996; Li and Dafalias, 2000). In the past few decades, within the framework of critical state soil mechanics (CSSM), the understanding of the soil behavior has become much more developed and extensive. Substantial knowledge on the mechanical behavior of granular materials has been gained mostly from the results of well-controlled laboratory testing on homogeneous specimens subjected to uniform stress and strains. As a conventional test, triaxial test is widely in use for characterizing the mechanical behavior of soils, and for determining the important soil parameters, and even for calibrating constitutive models for soils (Bishop and Henkel, 1962; Schofield and Wroth, 1968; Wood, 1990; Ishihara, 1996).

However, routine investigations can only provide the macroscopic response of soils, and information at the particulate level is scarce due to the lack of extensive microscopic measurements. The insufficient explanations of the observed macro-scale response are partially ascribed to the scarcity of the microscopic knowledge. As a particular interest, critical state (CS) is always an important subject of soil, and has attracted great research attentions over the years. Nevertheless, the microscopic response of granular soil in the CS is not clear, although the CS can be directly determined based on results from the

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laboratory tests.

This paper aims to present an alternative view on the granular material behavior using the discrete element method (DEM). A series of biaxial constant volume and drained tests are conducted, with varying initial densities and confining pressures. The simulated mechanical behavior of the granular materials is compared and discussed, based on those observed from the laboratory tests. Unlike the conventional laboratory tests, the information in the particulate level of this study is transparent, and the corresponding evolutions of microstructure during the loading process are captured and analyzed, including the response at the CS.

MODEL SETUP AND NUMERICAL IMPLEMENTATION

DEM is a numerical tool pioneered by Cundall and Strack (1979), and is capable of describing the micromechanical behavior of a particle assembly. In recent years, a commercial code particle flow code in 2D (PFC^{2D}) (Itasca Consulting Group Inc., 2005) has emerged as a popular and mature DEM program, and has been widely applied in research fields (Lobo-Guerrero and Vallejo, 2005; Wang *et al.*, 2007; Lu and McDowell, 2007). Generally, PFC^{2D} provides a platform for users to develop their own codes to resolve various problems. In this regard, the corresponding built-in program FISH is employed to implement the simulations in this study.

In the numerical simulation, all the particles are circular discs and the particle diameters range from 0.26 to 0.66 mm uniformly. According to ASTM, such a particle assembly can be treated as medium to fine sand. The numerical samples are generated by the expansion method. In this method, the initial diameters of the particles are reduced by a factor, such that all particles with reduced diameters are first created and fill up the constrained room. Once the particles have been created, their initial diameters of the particles are restored and an equilibrium state is achieved by cycling the particle assembly. A detailed description will not be elaborated here but can be referred to (Itasca Consulting Group Inc., 2005; Li, 2006; Yang, 2007) and so on. In this study, after considering the trade-off between the representiveness of simulated behavior and the computational cost, a sample dimension of 25 mm×25 mm is selected and treated as a representative elementary volume (REV), which consists of 3000 particles.

Once the sample is generated, the free stress state is not always satisfied. Any lock-in stresses should be released by simultaneously moving boundary walls, as to bring the specimen to a reference state with an isotropic confining stress of 10 kPa. Then a compaction procedure is followed which leads the particle assembly to the desired stress state. Biaxial compressive shear under drained condition can be proceeded by moving both the upper and lower boundary walls with a very slow loading rate while maintaining a constant horizontal stress (lateral confining stress), which is achieved by moving the lateral walls inwards or outwards as needed. The constant volume simulation is to guarantee no volume change during the course of shearing. Fig.1 illustrates a biaxial test sample with imposed boundary conditions and reference coordinate system.

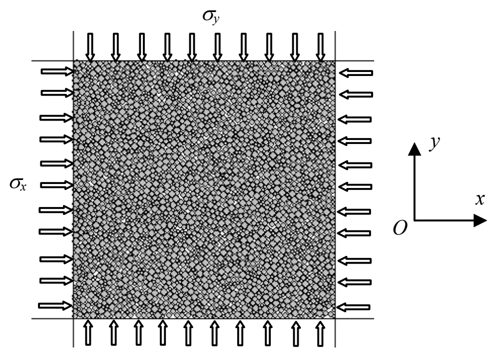

Fig.1 DEM model of a biaxial shear test

In this 2D analysis, the mean normal stress and deviatoric stress are expressed as $p=(\sigma_x+\sigma_y)/2$ and $q=\sigma_y-\sigma_x$, respectively, where σ_x and σ_y are principal values along x and y directions, respectively (Fig.1). All parameters used in the numerical simulation are those commonly used in literature or the default values of PFC^{2D}, which are summarized in Table 1. A linear contact model is adopted for DEM analysis in this study, as shown in Fig.2. Particularly, as suggested by Johnson (1985), the same stiffness in the normal and tangential directions of the particles is used. The wall's stiffness is assigned to be the same as that of the particles, while the friction between a wall and a particle is set to be zero, i.e., the boundary particles can move freely along the tangential direction of the walls.

Table 1 Parameters used in numerical simulations

Parameter	Value
Mass density (kg/m^2)	2600
Normal stiffness of particle/wall (N/m)	1.0×10^9
Tangential stiffness of particle/wall (N/m)	1.0×10^9
Particle/Wall friction	0
Damping parameter	0.7

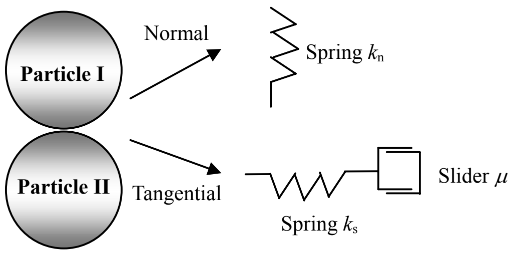

Fig.2 Linear contact model for DEM analysis

MACROSCOPIC RESPONSE AND CRITICAL STATE

Fig.3 shows the mechanical behavior of the granular assembly sheared under biaxial constant volume condition. All samples have the same initial density with a void ratio e=0.220, but with different confining stresses of 100, 200, 500 and 1000 kPa, respectively. The corresponding stress paths are presented in Fig.3a showing that all the samples exhibit contractive response firstly at the small shear strain, and then dilate, until the CS is reached after passing through the phase transformation (Ishihara *et al.*, 1975), which is known to be a typical sandy soil behavior. Fig.3b shows the results of the stress-strain curves, where axial strain ε_a is the strain along the y direction. Although a prominent distinction can be observed at the early stage of the shearing among various testing conditions, all the samples are sheared to and ended at an essentially common state, which is known as the CS. It is further noted from Fig.3c that the stress ratio q/p is more or less stabilized when the axial strain exceeds 10%, and falls into a narrow range of 0.56~0.58, known to be the CS stress ratio.

Fig.4 shows the counterpart of Fig.3 under drained condition, with the samples having different initial densities after being compressed to 500 kPa isotropically. It is seen that in Fig.4a, loose samples exhibit a hardening behavior, while dense samples tend to show strain-softening after reaching their peak states. However, an essentially identical CS is finally approached when the samples are subjected to large deformations. An alternative view on the CS is shown in Fig.4b suggesting that a common state with identical deviatoric stress q and void ratio e may be attainable, irrespective to whether the samples being contractive or dilative before that state. A similar observation to the constant volume test on the stress ratio is shown in Fig.4c, which shows that the CS stress ratio ranges between 0.57 and 0.59. This suggests that the stress ratio at CS should be independent of the test modes (drained or constant volume).

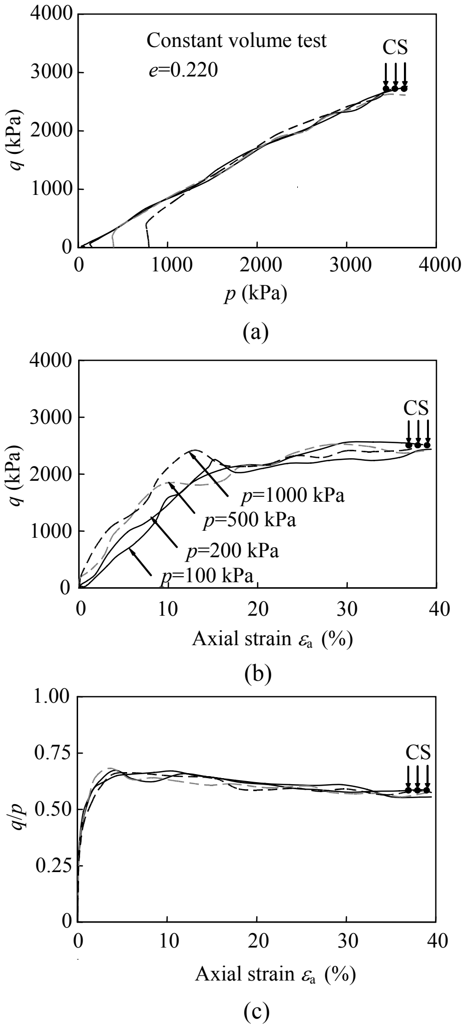

Fig.3 Typical macroscopic behavior for constant volume test under various initial confining pressures. (a) q~p; (b) q~ε_a; (c) q/p~ε_a

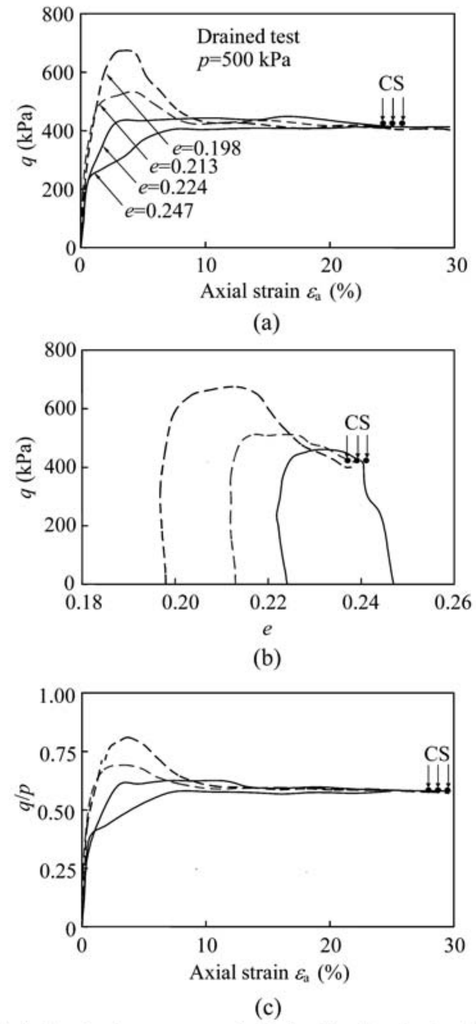

Fig.4 Typical macroscopic behavior for drained test under various initial densities. (a) q~ε_a; (b) q~e; (c) q/p~ε_a

It is known that the CS is an ultimate state of a material, and can be expressed in the p-q-e space by the following equation

$$\frac{\partial p}{\partial \varepsilon_q}=\frac{\partial q}{\partial \varepsilon_q}=\frac{\partial e}{\partial \varepsilon_q}. \tag{1}$$

Eq.(1) shows that at the CS, no changes are allowable except the deviatoric strain ε_q. It has been shown that the CS stress ratio q/p is actually independent of the test modes, and the CS line in the p-q plane is a straight line originating from the origin with a slope of the CS stress ratio (0.56~0.59). The CS line in the e-p plane can be determined from the tests presented above, together with some extra tests for integrality. In Fig.5, the triangle symbols denote the CS evaluated from the biaxial compression tests including constant volume and drained tests, and these symbols can be approximated by a straight line using the least squares fitting.

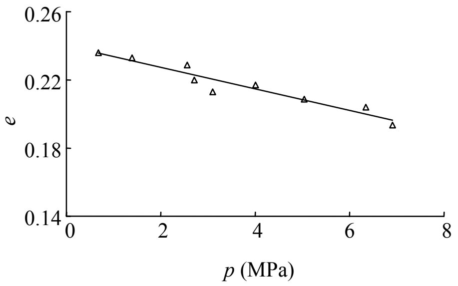

Fig.5 Critical state line of biaxial compression in *e-p* plane

MICROSCOPIC OBSERVATION

The microstructure changes can be represented through the coordination number (CN) and contact unit normal during the loading process. CN is a scalar quantity that characterizes the average contacts of each particle among the whole assemblage. The contact unit normal is a spatial vector that denotes the contact direction among neighboring particles. The contact unit normal can be characterized by a pair of unit vectors $\boldsymbol{n}$ and $-\boldsymbol{n}$, paralleled but with opposite directions (Oda, 1999). It has been shown that the directional distributions of contact unit normal $E(\varphi)$ can be expressed by the intensity Δ and preferred orientation φ_0. The function of $E(\varphi)$ can be written explicitly in the form of

$$E(\varphi)=1/[2\pi(1+d_{ij}n_in_j)]=1/\{2\pi[1+\Delta\cos 2(\varphi-\varphi_0)]\}, \tag{2}$$

where φ denotes the orientation of the micro-quantity while φ_0 denotes the principal directions, measured with respect to horizontal axis, d_{ij} is a second-order deviatoric tensor, and n_i and n_j are unit normals. The parameters Δ and φ_0 can be obtained through the following equation

$$\Delta=\sqrt{d_{11}^2+d_{12}^2},\ \ \varphi_0=\frac{1}{2}\mathrm{arc}\tan(d_{12}/d_{11}). \tag{3}$$

A detailed derivation of this section can be found in APPENDIX.

To investigate the microstructure change during the biaxial shear, the constant volume tests are further analyzed afterwards. The evolutions of CN during the shear are illustrated in Fig.6. It is seen that, in general, CN value varies as the shear proceeds. However, at the CS with larger strains, CN values of various tests merge together and become a constant as shown in Fig.6.

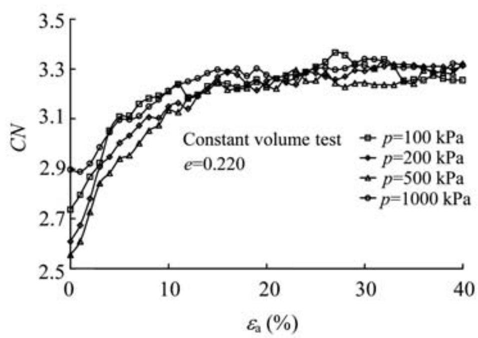

Fig.6 Evolution of CN during the biaxial shear under various initial confining pressures

Fabric anisotropy is a general feature for granular materials. During the course of the shear, the initial anisotropy of the granular assembly may be subjected to significant changes, which are termed 'induced anisotropy', to distinguish with the inherent anisotropy (Arthur and Menzies, 1972). The evolutions of the anisotropy can be illustrated by the distributions of the contact unit normal. Fig.7 shows the distributions of the contact unit normal at various loading stages for a particulate test (e=0.220, p=100 kPa) under the constant volume condition. It is evident that before the shearing (Fig.7a denoted by 0 axial strain), the initial distribution of the contact unit normal is essentially isotropic, indicating that the expansion preparation method may yield an isotropic sample under an isotropic stress state. However, as the shearing begins, the contact unit normals are redistributed, and the biaxial shear gradually drives the granular sample to a more anisotropic state, as can be seen from the corresponding distribution patterns at different shearing stages: 10%, 20% and 40% axial strains. The initial anisotropy of the contact unit normal is gradually destroyed during the course of the shear, and the induced anisotropy is developed accordingly.

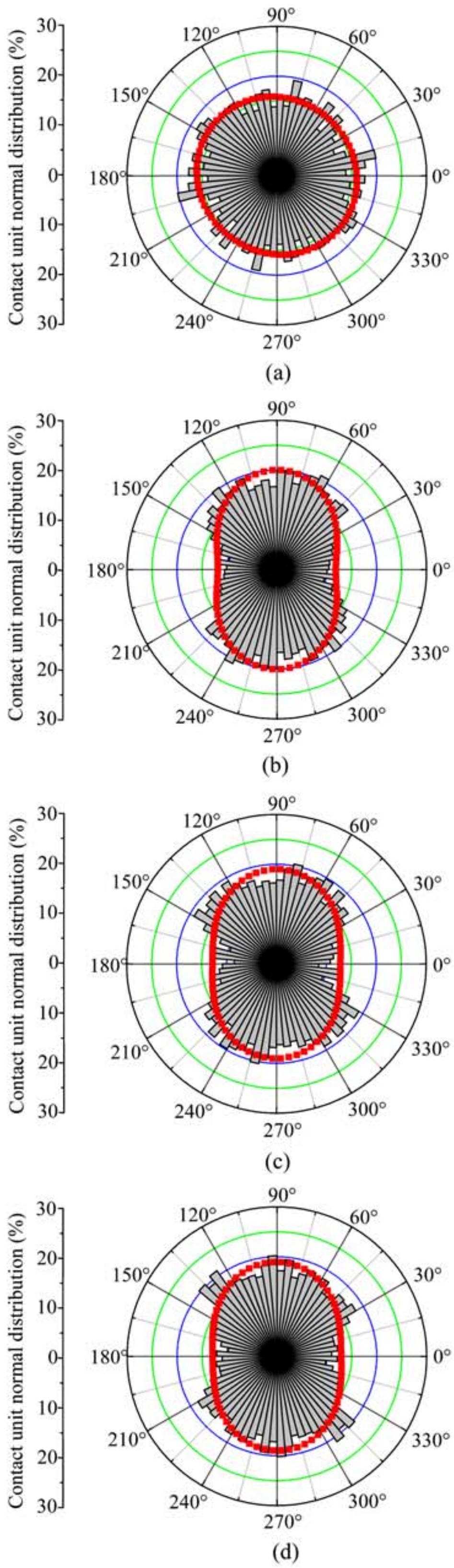

Fig.7 Contact unit normal distributions at various shearing stages. (a) 0; (b) 10%; (c) 20%; (d) 40%

A more detailed evolution of the anisotropy of the tests described in Fig.3 is given in Figs.8 and 9, in terms of two parameters Δ and φ_0, respectively, as suggested by Eq.(2). It is found that though different confining pressures are applied in the test with the same initial density (e=0.220), the microstructure evolution follows the same pattern. It is seen from Fig.8 that the parameter Δ prior to the peak increases as the shear strain. It drops gradually until the CS is reached. The increase in Δ also suggests that the sample is sheared from the isotropic state to a more anisotropic one, which is evidenced from the illustrations in Fig.7. Fig.9 shows the evolution of the preferred orientation φ_0 for the contact unit normal distributions among all constant volume tests. It is seen that the preferred orientation is coincidental with the major principal stress direction σ_1 (vertical direction), which is supported by ample experimental observations, that the concentration of the contact unit normals towards the major principal stress direction, such as Drescher (1976) and Oda *et al.*(1980; 1982). But it is generally not true for the non-proportional loading like the tests involving rotation of the stress direction, in which the coordinates of the material's fabric may differ from the principal stress axis. It is further concluded from Figs.8 and 9, that at CS the test samples (Fig.3) may have a unique distribution (anisotropy) in contact unit normal.

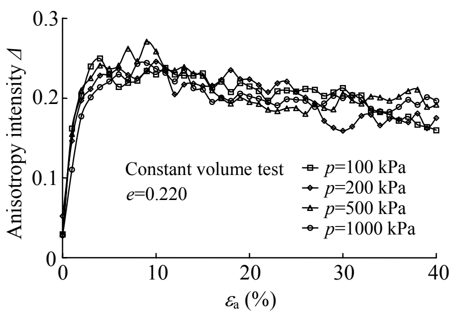

Fig.8 Evolution of anisotropy intensity for contact unit normal orientation

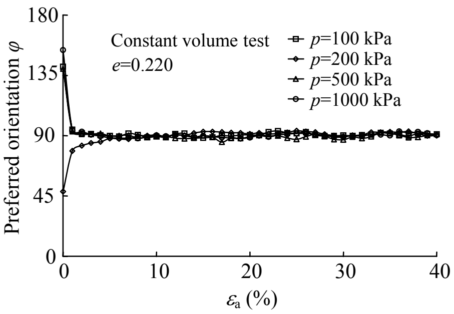

Fig.9 Evolution of preferred orientation for contact unit normal distribution

CONCLUSION

In this paper, granular material behavior is investigated by the numerical approach with the aid of DEM. Different from the experimental approach, the numerical method has the advantages of providing the mechanical behaviors of granular assembly in both the macro- and micro-scales. A series of biaxial compression tests on the samples with different initial confining pressures and initial densities, under both the constant volume and drained conditions are carried out. The conclusions are summarized as follows:

(1) DEM successfully simulates the typical granular material behavior in the biaxial compression mode, as observed from the experimental tests.

(2) The CS defined in the soil mechanics can be determined through such numerical tests. The CS line is shown to be a proximately linear relationship between the mean normal stress p and void ratio e.

(3) Particulate-scale analysis suggests that during a biaxial shear, considerable microstructure changes occur. The microstructure of an initially isotropic sample is destroyed and yields a more anisotropic structure (induced anisotropy).

(4) The analysis on samples sheared under constant volume conditions, with the same initial densities (e=0.220) under varying confining pressures, suggests that the distribution in the contact unit normal follows the same pattern at the CS, which is defined originally in the continuum level.

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APPENDIX: MICRO-QUANTITY INTERPRETATION

The geometrical packing of granules with associated voids contributes to the general feature—fabric anisotropy for granular materials. Generally, the quantities or variables in the micro-scale are used to quantify the anisotropic property of granular materials. Quantities like particle orientation and contact unit normal can be characterized by a pair of unit vectors $\boldsymbol{n}$ and $-\boldsymbol{n}$, with opposite directions, such that a fabric tensor can be expressed in the form (Oda, 1999)

$$F_{ijlm\cdots} = \frac{1}{2N}\sum_{k=1}^{2N} n_i^k n_j^k n_l^k n_m^k \cdots, \qquad \text{(A1)}$$

where $2N$ is the total number of the measurements, the superscript k denotes the kth unit vector among $2N$, and $\boldsymbol{n}_i^k$ $(i=1,2,3)$ are direction cosines of the unit vector n^k with respective to the reference axes x_i (i=1, 2, 3) in a Cartesian coordinate system.

In the meanwhile, a density function $E(\boldsymbol{n})$ also can be used to characterize the directional properties of micro-quantities and can be expressed as

$$E(\boldsymbol{n}) = E_0(1 + d_{ij}n_i n_j + d_{ijlm}n_i n_j n_l n_m + \cdots), \qquad \text{(A2)}$$

where E_0 is a mean value of the density over the directions of the space and satisfies the condition of unity for all directional summation, d_{ij} and d_{ijlm} are the second order and the fourth order deviatoric tensors, respectively, measuring the deviations from the corresponding isotropic distribution. Alternatively, it is also convenient to use the deviatoric tensors to describe the directional distribution of micro-quantities. By using the density function defined in Eq.(A2), Eq.(A1) can be rewritten into an integral form

$$F_{ijlm\cdots} = \int_{\boldsymbol{n}} E(n) n_i n_j n_l n_m \cdots \mathrm{d}\boldsymbol{n}. \qquad \text{(A3)}$$

Noting the deviatoric and symmetric property of the deviatoric tensor d_{ij}, the corresponding fabric tensor F_{ij} can be further expressed by substitution of Eq.(A2) into (A3):

$$F_{ij} = 1/(3\delta_{ij}) + 2/(15 d_{ij}),\ \text{for 3D case}, \qquad \text{(A4)}$$

$$F_{ij} = 1/(2\delta_{ij}) + 1/(4 d_{ij}),\ \text{for 2D case}, \qquad \text{(A5)}$$

where δ_{ij} is the Kronecker delta. Eq.(A5) establishes a relationship between the fabric tensor F_{ij} and the deviatoric fabric tensor d_{ij}. Since one may directly evaluate the fabric tensor F_{ij} based on Eq.(A1) by using discrete measuring data, the deviatoric fabric tensor d_{ij} can be captured accordingly.

In the 2D case, for quantities only having information in direction (no information in magnitude), such as particle orientation, contact unit normal and branch vector orientation, etc., the directional distribution in terms of the density function can be written as

$$E(\varphi) = E_0(1 + d_{ij}n_i n_j) = E_0[1 + \Delta\cos 2(\varphi - \varphi_0)], \quad \text{(A6)}$$

where φ measures the orientation angle of an interested quantity with respect to the horizontal axis, ranging from 0° to 360°; E_0=1/(2π) designates an isotropic distribution part; and Δ and φ_0 are two parameters characterizing the intensity and principal direction of the anisotropic distribution of a particular quantity, which can be calculated through the components of d_{ij}, d_{11} and d_{12} (only two is sufficient in expressing the tensor d_{ij} because of its deviatoric and symmetric properties), using the following relations:

$$\Delta = \sqrt{d_{11}^2 + d_{12}^2} \text{ and } \varphi_0 = \frac{1}{2}\arctan(d_{12}/d_{11}). \quad \text{(A7)}$$

It is noted that Eq.(A6) gives the directional distribution of the quantities only having orientational information, while Eq.(A7) designates the anisotropy intensity and principal direction of such a distribution.