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**DEM modeling of the one-dimensional compression of sands incorporating a statistical
particle fragmentation scheme**

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Abstract

This paper presents a novel framework of modeling crushable granular materials under mechanical loadings based on the discrete element method (DEM). The framework is featured with the construction of the one-to-one model in which every particle in a physical experiment has its own numerical twin and allows the modeling of irregular shaped fragments during the continuous breakage process. First, image processing techniques and spherical harmonic (SH) analysis were adopted, respectively, to segment and label particles and to construct a one-to-one model mathematically in DEM. Then, a particle crushing criterion based on the maximum inter-particle contact force was used to predict the crushing events, showing fitting results that agreed very well with a large number of single particle crushing tests. Next, a statistical approach for the generation of particle fragmentation modes of a given type of sand particles based on the principal component analysis (PCA) was proposed. The aim of the PCA was to analyze the statistical trends of the coefficient matrix, which was composed of the SH coefficients of all the particles involved in the analysis. Finally, a successful modeling of a particle crushing event was achieved by replacing the particle, which was judged by the crushing criterion to undergo crushing, with a few sub-particles chosen randomly from a specific fragment template constructed using the micro-computed tomography (micro-CT) data.

Keywords

Particle fragmentation scheme, one-dimensional compression, discrete element method, statistical particle reconstruction, principal component analysis

1 Introduction

Particle breakage influences the properties of granular materials at elevated stress levels, which occurs in many geotechnical structures including offshore piles, rock-fill dams and railway ballast (e.g., Nakata et al. 2001; Altuhafi and Coop 2011; McDowell and De Bono 2013), etc. A particle crushes into multiple pieces when the internal stress exceeds its failure strength. The crushability of soil particles depends on particle morphology, microstructure, and mineralogy (e.g., Zhao et al. 2015; Karatza et al. 2019), and packing features, such as void ratio and grading (e.g., Nakata et al. 2001; Coop et al. 2004). Particle breakage will change particle size, shape, and material fabrics, including coordination number (CN) and particle contact distribution.

In-situ X-ray characterization of single particle crushing tests and high-pressure compression tests reveal the evolution of particle shape under external loading (Zhao et al. 2015; Zhao et al. 2019). The fragments tend to be angular due to the existence of fracture planes. Particle shape, in turn, influences the mechanical properties of granular materials, e.g., compressibility, shear strength, and crushability (e.g., Guo and Su 2007; Rousé et al. 2008; Tsomokos and Georgiannou 2010; Altuhafi and Coop 2011). Elongated particles are prone to experience bending failure, while angular particles have higher stress concentration at corners (Zhao et al. 2019).

Discrete element modeling has been adopted to investigate the influence of particle breakage in soil mechanics. DEM models crushable particles through agglomerates or discrete fragmentation methods. The agglomerates method glues element particles with 'cement-like' bonds, which break under certain stress levels (e.g., McDowell and Harireche 2002; Cheng et al. 2003; Potyondy and Cundall 2004; Wang and Yan 2013; Laufer 2015). Similar to the agglomerates method, the combined finite discrete element method (FDEM) simulates the inter particle contacts using DEM

approach and simulates particle fragmentation based on finite element method (FEM) (e.g., Latham et al. 2008; Ma et al. 2017; Wei et al. 2019; Zhou et al. 2020). The agglomerates method avoids defining failure criteria and fragmentation patterns. However, hundreds of elementary spheres are needed to represent the three-dimensional (3D) geometry of each particle, and the computational cost for the intra-agglomerates contacts limits the total number of particles included in a simulation.

In contrast, the discrete fragmentation method artificially replaces crushing particles with smaller fragments based on given particle breakage criteria and fragmentation pattern (e.g., Åström and Herrmann 1998; Lobo-Guerrero and Vallejo 2005; De Bono and McDowell 2014). The particle breakage criterion depends on a number of factors including particle geometric and physical properties and inter-particle contact conditions. The fragmentation pattern typically comprises of a group of fragments conforming to a specific size distribution (e.g., Ben-Nun and Einav 2010; Ciantia et al. 2015; Zhou et al. 2020). However, these assumptions are oversimplified for considering irregular shapes of fragments. Therefore, the application of the discrete fragmentation method to the crushing of real sand particles with irregular shapes is still a challenge.

In a previous study of the authors (Wu et al. 2020), a 3D DEM model of a mini-triaxial sand specimen which incorporates the realistic particle morphology of every sand particle acquired from micro-CT scanning has been established. On the basis of that study, the current paper aims to take a step further to enhance the capability of the DEM model by including the modeling of particle breakage throughout the loading process. The major thrust of this work is to propose a statistical particle fragmentation scheme to generate irregularly shaped fragments following the successive particle crushing events, utilizing the micro-CT data of actual crushed particles within a mini-

specimen subject to one-dimensional (1D) compression. The simulation results show that the macroscopic (e.g., stress-strain) and particle-scale behavior (e.g., evolutions of particle size) agree very well with the results obtained from the micro-CT experiment. A particularly interesting aspect of the micromechanical analysis is extracting of the major contact force chain (MCFC) and its sustaining granular skeleton (SGS) from the DEM simulation and then comparing the SGS with its counterpart derived from the physical specimen, an analysis that cannot be done by using DEM or micro-CT alone.

2 Micro-CT testing of 1D compression of sand

The micro-CT results used in this study were reported by Zhao et al. (2019), who performed 1D compression of mini-samples of Leighton Buzzard sand (LBS) with in-situ CT scanning. The sample had an equal diameter and height of 6 mm and contained about 308 grains with a size range of 0.6 ~ 1.18 mm. The sample was compressed at a constant rate of 1.8 mm/h, and the compression was paused at vertical stress levels of 1 MPa (strain 0.75%), 10 MPa (strain 4%), 14 MPa (strain 5%), 19 MPa (strain 7%), and 28 MPa (strain 13%), corresponding to Scans 1-5 respectively, to acquire the CT images of all sand particles.

A series of image processing and mathematical modeling techniques were adopted to segment individual particles and to reconstruct realistic particle shapes. First, the *watershed* algorithm (Beucher and Lantuejoul 1979) was used to separate individual particles. Then, the individual particles were labeled with different integers. The binary image with only two intensity values (i.e., 255 and 0) is shown in Fig. 1(a), in which grains are labeled with 0, and voids are labeled with 255. Fig. 1(b) is the image of the labeled particles after using the 3D *watershed* algorithm. Next, the SH function was adopted to reconstruct the irregular particle shapes. Lastly, the *scripting language* was used to sort the particles according to the magnitude of volume to be incorporated into

DEM for the convenience of one-to-one mapping.

Following the image processing, a comprehensive analysis of the particle breakage behavior through the use of a number of quantitative descriptors, including fractal dimension, specific surface area, and CN, etc., was made to reveal the linkage between particle breakage and macroscopic compression behavior. More details about the micro-CT experiments, image processing, and data analysis can be found in Zhao and Wang (2016) and Zhao et al. (2019).

3 DEM method

3.1 Particle breakage criterion

The first step to model the real particle breakage behavior is to select a physically sound particle breakage criterion. In the literature, a number of particle breakage criteria, such as the maximum contact force criterion (Hanley et al. 2015; Marketos and Bolton, 2007), the mean and major principal stress criterion (De Bono and McDowell 2016), the octahedral shear stress criterion (McDowell and De Bono 2013), the maximum tensile stress criterion (Lobo-Guerrero and Vallejo 2005) and the rigorous breakage criterion to represent failure of grains isolated between platens or within granular masses (Ciantia et al. 2015 and Ciantia et al. 2019a, 2019b) based on the modeling of elastic stress redistribution by Russell et al. (2009) have been proposed to predict particle crushing in DEM modeling. Among others, Zhu and Zhao (2019a) found that the maximum contact force criterion, which dictated the occurrence of particle crushing when the maximum contact force reached a threshold, was more suitable for predicting particle crushing than others when a particle had multiple contacts with neighboring particles. Their results indicated that the crushing threshold obtained by the maximum contact force criterion was not apparently affected by the CN and showed a relatively good consistency under different loading conditions. Compared

to the maximum contact force criterion, the major advantage of the rigorous breakage criterion proposed by Ciantia et al. (2015) considers the stiffness of the grains and of the platens, because when there is a large difference between the two stiffness values, there may be a certain degree of error in predicting a particle breakage event. However, such an issue is not the main concern of the current study, since in the experiment the loading platens are made of ceramic whose stiffness is close to that of sand and has a low density to reduce the X-ray attenuation contrast. Therefore, the maximum contact force criterion was adopted in this study to predict particle crushing.

To study the crushing of rocks between two platens, Jaeger (1967) proposed the following expression to define the characteristic tensile strength of particles:

$$\sigma = \frac{F}{d^2}, \quad (1)$$

where F is the crushing load, d is the initial diameter of the particle, and σ is the characteristic tensile strength. Eq. (1) has been widely used to determine the crushing strength of sand particles (e.g., Nakata et al. 1999; McDowell and Amon 2000; Nakata et al. 2001). In describing the statistical variation of particle crushing strength, Nakata et al. (1999) modified the Weibull equation (Weibull 1951) by considering particle size as follows:

$$P_s(d) = \exp \left[- \left(\frac{d}{d_0} \right)^3 \left(\frac{\sigma}{\sigma_0} \right)^m \right], \quad (2)$$

where m is the Weibull modulus only depending on the material, and σ_0 is the characteristic crushing stress corresponding to 37% of survival probability for the particles with a characteristic diameter d_0 .

In order to determine the values of σ_0 and m of LBS particles, single particle crushing tests were conducted on 147 LBS particles with a size range of 0.6 ~ 1.18 mm (same as Zhao et al. 2019). The Weibull distribution of particle survival probability P_s

vs. particle crushing strength σ is shown in Fig. 2. The distribution is plotted in two formats, namely, $\ln[\ln(1/P_s)]$ vs. $\ln(\sigma/\sigma_0)$ shown in Fig. 2(a) and P_s vs. σ shown in Fig. 2(b). The values of σ_0 and m are determined to be 50 MPa and 3.2, respectively, for LBS particles based on the approximately linear correlation. Following Hanley et al. (2015) and Zhu and Zhao (2019b), the correlation of P_s vs. σ in Fig. 2(b) can be approximated as:

$$\sigma = \sigma_{0,d} \frac{U(0,1) - b_s}{a_s}, \quad (3)$$

where $U(0,1)$ is a random real number between 0 to 1 generated by a uniform distribution seed generator; a_s and b_s are the slope and intercept of the linear fit (Fig. 2(b)), respectively, determined to be -0.77 and 1.25, respectively. Following Nakata et al. (1999), the characteristic strength $\sigma_{0,a}$ and $\sigma_{0,b}$ for particles a and b with any diameter d_a and d_b can be described as:

$$\frac{\sigma_{0,a}}{\sigma_{0,b}} = \left(\frac{d_a}{d_b} \right)^{-\frac{3}{m}}. \quad (4)$$

Combining Eqs. (1), (3) and (4), the crushing force acting on the particle with a size d can be obtained as:

$$F = \sigma_0 \frac{U(0,1) - b_s}{a_s} \left(\frac{d}{d_0} \right)^{-\frac{3}{m}} d^2. \quad (5)$$

Eq. (5) was used to generate the crushing strength data of all particles to be used in the DEM simulation. It shall be noted that the above approach of calculating the particle crushing strength involving a linear approximation of the particle survival probability function was also used by a number of authors (e.g., Wang and Yan 2013; Hanley et al. 2015; Zhu and Zhao 2019b).

3.2 Statistical particle fragmentation scheme

3.2.1 Statistical reconstruction of a virtual particle database with spherical harmonics

Spherical harmonics (SH) are a complete set of orthogonal functions used to represent the multiscale morphology of a particle surface. The orthogonal functions are used to expand the polar radius of every vertex at the particle surface from a unit sphere and to calculate the associated SH coefficients. The obtained SH coefficients therefore constitute a database of the morphological genes of all the input particles. The aim of this task is to statistically generate a database of virtual particles based on the SH coefficients of a given group of sand particles. Note that the virtual particles do not exist actually but possess realistic morphological features that are inherited from the input particles.

Following Zhou et al. (2015), this task can be performed by using the principal component analysis (PCA) of SH in three steps. First, a group of input particles were analyzed with SH analysis to obtain their SH coefficients. Second, the PCA was made to decompose these SH coefficients into the principal component vector $\mathbf{P}$ of SH coefficients and the corresponding variance coefficients c_v . Finally, the SH descriptor $\hat{\mathbf{c}}$ of a virtual particle can be obtained as:

$$\hat{\mathbf{c}} = \bar{\mathbf{c}} + \mathbf{p}(x_1) \cdot c_v(x_1) \cdot x_2, \quad (6)$$

where $\bar{\mathbf{c}}$ is the mean vector of given SH descriptor; $x_1 \in [1, 2, 3]$ refers to the coordinate axis x , y and z ; $c_v(x_1)$ is the variance coefficient; and $x_2 \in [-3.0, 3.0]$ is a random real number that satisfies the Gaussian distribution. The above PCA-based SH analysis was made to generate a particle database containing a total number of 9,000 virtual particles based on micro-CT data of the initial 308 LBS particles before the compression test. A more detailed description of the above method can be found in Zhou et al. (2015) and Zhou and Wang (2017).

3.2.2 Generation of virtual fragment templates

This paper aims to use the discrete fragmentation method to reproduce the sand breakage behavior in the 1D compression test. The discrete fragmentation method allows replacing crushed particles with smaller fragments based on the given particle breakage criterion and the fragmentation pattern. Unlike most previous approaches for simulating sand particle breakage using spherical fragments, we create 5 templates of fragments using CT data of crushed particles obtained at different stages of the test. The fragment templates are composed of a small assembly of fragments with irregular shapes. For the current DEM study, it is necessary to refer to the experimental data to carry out the DEM simulation.

The novel feature of this study lies in generating 5 templates of virtual fragments, with each template comprising of 100 virtual fragments except for Template 1, from the particle database corresponding to increasing fragmentation degrees at the 5 scans during the compression test. Template 1 is composed of 308 original particles gained from Scan 1. Virtual fragments refer to the artificial fragments generated by the PCA-based SH analysis, which do not exist in the real world. In the shearing process, any particle whose maximum contact force satisfying the particle breakage criterion will be ‘instructed’ to crush, and the current vertical strain will be outputted as well. Then, a template of virtual fragments is selected according to the macroscopic vertical strain obtained at the moment. For instance, if the vertical strain is below 0.75%, Template 1 will be invoked. If the vertical strain is between 0.75%~3.9%, Template 2 will be invoked. Similarly, Template 3 and 4 will be invoked, respectively, if the vertical strain is between 3.9%~5.4% and 5.4%~7.2%. If the vertical strain is greater than 7.2%, Template 5 will be invoked. A number of fragments are randomly selected from the invoked template, and their size is adjusted following the AG/SAG breakage

probability model (Bruchmüller et al. 2011). In the particle replacement process, an approximate target porosity of 0.36 (corresponding to a very dense 3D packing) is set instead of specifying the number of fragments to be generated.

The detailed procedure to generate Templates 2, 3, 4 and 5, using Template 2 as an example, is described as follows. Fig. 3 illustrates the process of the virtual template generation. The same procedure applies to the generation of other templates. Firstly, the cumulative frequency distributions (CFD) of two particle shape parameters, namely, aspect ratio (AR) and sphericity (S) of all the crushed particles from Scan 2 (Zhao et al. 2019) were plotted and each curve was uniformly divided into 25 equal intervals, according to the value of AR or S . 25 intervals were used in this study to balance the computational efficiency and accuracy. The percentage of fragments in each interval represented by the average value of the concerned shape parameter within that interval can then be easily measured from the CFD curve. The total number of fragments is set to 100 for each template and so the number of fragments within each interval can be simply calculated by multiplying its percentage by 100. Secondly, values of AR_i and S_j (i and j are integers from 1 to 100; i and j must take every value from 1 to 100 once and only once) were randomly combined to determine the shape characteristics of the 100 fragments, which were considered to be representative of the morphological features of all crushed particles acquired from Scan 2 in the physical test. Thirdly, an advanced sieve analysis was made on the particle database to find the particles that have combinations of shape parameters matching those designated above. In detail, for a designated combination (AR_i, S_j), the particles with AR values close enough to AR_i (within a given threshold) were selected first from the particle database. Then, the particle with S value closest to S_j was selected from the short list. Our results show that a threshold value (i.e., the difference between the candidate and target values

of a concerned shape parameter) of 0.001 can lead to a great match with a high accuracy.

In this study, the rigid block feature of PFC^{3D} v.6.0 (Itasca Consulting Group 2018), instead of the clumping feature used by Wu et al. (2020), was used to model irregularly shaped particles for the following two reasons. First, a rigid block is a 3D polygonal entity that represents the surface of an irregular particle using the convex hull and allows only one contact between two rigid blocks, with the contact location being placed at the centroid of the overlap region (i.e., area in 2D and volume in 3D). While for the clumping feature, the irregular particle shape is approximated by a group of overlapping spheres, and multiple contacts may exist between two clumping particles. Since we are not performing simulations with one-to-one mapping (as done by Wu et al. (2020)) that accurately reproduces the particle morphology of every single particle in this study, the rigid block has an advantage of reducing the number of contacts between particles, which is beneficial to the computational efficiency. Second, using the rigid block feature to simulate the successive particle breakage events can also avoid the unphysical behaviors such as local stress concentration and redistribution, because there will be little overlaps among zero-porosity rigid blocks (and with their neighboring particles as well) that are employed to fill the convex hull and replace the original particle.

Fig. 4 compares the distributions of the particle shape parameters from Template 2 and Template 5 with the experimental measurements from Scan 2 and Scan 5, respectively. It is evident that an excellent agreement exists between all the predicted and measured curves. This result indicates that the proposed statistical fragmentation scheme can fully meet the requirement of creating fragments that are statistically representative of the real shapes of crushed sand particles.

3.3 DEM simulation

This study adopts the three-dimensional particle flow code PFC^{3D} (Itasca Consulting Group 2018) to perform DEM simulations. The model reproduces the initial configuration of the sample including one-to-one mapping of all 308 grains enclosed within a cylindrical container with an equal diameter and height of 6 mm. Following the physical testing procedure of Zhao et al. (2019), the sample was confined by the fixed cylindrical wall and bottom platen and compressed vertically by moving the top platen downward at a constant rate of 1.8 mm/h.

All the SH-reconstructed particles were represented by rigid blocks. The rigid block is a closed, convex and manifold polyhedron that is composed of triangular facets, which allows the modeling of non-spherical objects when the shape is of importance. During the shearing process, the rigid blocks do not have any degree of edge rounding. The Gilbert–Johnson–Keerthi algorithm (Gilbert et al. 1988) is used to determine the overlap state of two closed, convex objects by introducing the concept of the Minkowski difference, which is a convex hull constructed from a set of vertices. For instance, if object A has M vertices on its exterior surface and object B has N vertices on its exterior surface, then the convex hull with $M * N$ vertices can be constructed as the Minkowski difference for the convex objects A and B, where $M * N$ vertices can be obtained by subtracting the entire set of vertices (represented by vectors) on object A from the entire set of vertices (represented by vectors) on object B. If the coordinate origin is within the Minkowski difference, the two objects overlap. The contact force can be calculated according to the detected overlap distance and the pre-defined contact model.

Fig. 5 compares the initial samples from the DEM model and the micro-CT test. Different colors are just used to represent different particles. The Hertz-Mindlin contact model is adopted in the simulations, and the micro-parameters used in the DEM

simulations are listed in Table 1. The choices of the microparameter values largely followed Wu et al. (2020) and Zhou et al. (2016) and then were fine-tuned by calibrating the model performance against the physical test results. Note that a local non-viscous damping coefficient of 0.2 was used in the DEM model in order to dissipate kinetic energy. Because without real experimental data, it is difficult to determine which value of the damping coefficient will produce over-damping, non-physical dissipation behavior. Besides, as reported by Wang and Yan (2012), changes in damping coefficient have very little influence on the material fabric evolution process which mainly influences the mechanical behavior of granular material. And using a higher value of damping coefficient may exaggerate the role of damping dissipation in the shearing process. For the current quasi-static simulations, it is more justified to use a low value of the local damping coefficient, which is less likely to overshadow the role of friction dissipation in the mechanical behavior of crushable soils.

The whole simulation test is conducted through calling 3 algorithms, in which Algorithm 1 is the main algorithm controlling the 1D compression test, Algorithm 2 is a subroutine called to invoke a specific fragment template and Algorithm 3 is another subroutine called to perform the replacement of crushed particles.

Table 1 DEM parameters for the 1D compression test

Sample parameters	Value
Size: height $\times$ diameter, mm	6×6
No. of rigid blocks	308
Contact model	Hertz–Mindlin
Friction coefficient	0.5
Shear modulus, GPa	29
Poisson's ratio	0.15
Local damping coefficient	0.2
Density, kg/m ³	2650

In Algorithm 1, particle breakage is checked every 100 timesteps and any particle whose maximum contact force satisfying the particle breakage criterion (Eq.

(5)) will be recorded and 'instructed' to crush in the next step. Specifically, Algorithm 2 is called to select a template of virtual fragment according to the macroscopic vertical strain of the specimen obtained at the moment. Then, Algorithm 3 is called to represent the target particle with a convex hull (Goshtasby and Stockman 1985; Zhao and Wang 2016) and randomly select fragments from the invoked template. The size of selected fragments is adjusted following the AG/SAG breakage probability model (Bruchmüller et al. 2011) to achieve an approximate target porosity of 0.36 (corresponding to a very dense 3D packing) within the convex hull after a local re-equilibrium is achieved. According to Narayanan and Whiten (1988), t_{10} (the progeny percent passing one tenth of the initial mean particle size and set to 10% in this study) is closely related to other points on a family of size distribution curves, t_n , defined as the cumulative percentage passing a given fraction of the initial size. The breakage behavior is affected by many factors like stress level, material property and particle size, etc., so that the consideration of these factors by the model would increase the simulation complexity and cost. Besides, considering a spatial distribution of fragments would lead to a considerable amount of artificial mass loss. Therefore, a random distribution of fragments has been adopted. Such a practice has also been adopted by many other authors for investigating the breakage behavior of spherical brittle particles (e.g., Bruchmüller et al. 2011; Zhou et al. 2016; Cil and Buscarnera 2016).

In this study, the average ratio of the unbalanced force was used to assess how far a system is from an equilibrium state (Itasca Consulting Group 2018). During the dynamic equilibrium process, Newton's second law is used to determine the motion of each particle arising from the contact and body forces acting upon it, while the force-displacement law is used to update the contact forces arising from the relative motion at each contact. The calculations performed in DEM alternate between the application

of Newton's second law to the particles and the force-displacement law at the contacts. These steps are iteratively performed until the termination condition (average ratio of unbalanced force $< 1e-5$) is satisfied. The above steps are performed iteratively until all the crushed particles are replaced. It is noted that the above particle replacement procedure will result in a certain amount of mass loss for each crushed particle. However, the accumulated mass loss at the end of simulation is within 5%, as will be shown later. The issue of mass loss in DEM simulation of particle breakage has also been reported by other authors (e.g., Ciantia et al. 2015; Lobo-Guerrero and Vallejo 2005; De Bono and McDowell 2014) and found to not show a significant effect on the macro-mechanical behavior of granular soils due to the minor role of fine particles in sustaining and transmitting the MCFC within the granular system (Török et al. 2005).

4 Simulation results

The simulation was performed on a workstation with Intel Xeon Gold 6154 processors (3.0 GHz, Skylake-SP) with 18-core $\times$ 2-CPU and 192 GB main memory. The computational efficiency primarily depends on the number of rigid blocks and the stored data. With a timestep of $1e-4$ s, the computation time used for a complete simulation is about 78 hours. In order to raise the computational efficiency so that the simulation can be completed within a reasonable timescale, the particle density scaling (Thornton 2000) was adopted in this study, in which the particle density was scaled up by a factor of 10^9 . With such a setup, the critical timestep is about $4e-4$ s, so we set the timestep to be $1e-4$ s.

Fig. 6 shows an overall agreement between the load-deformation relationships obtained from the simulation and the experiment. In the small strain (0%–3%) range, the agreement is almost perfect, indicating that the complex contact interactions and stiffnesses, which are mainly controlled by the irregularities of the particle surfaces, are

well reproduced. Such close agreement may not be achieved when the particles are shaped as spheres and ellipsoids, among others. Two stages of larger axial strains are defined: 3%–5% and 5%–13%. During the 3%–5% stage, the stress produced by the simulation slightly exceeds that of the experiment, indicating a slight difference in particle kinematics and crushing events. During the 5%–13% stage, the two responses are matched almost perfectly again. The sample yielded around 10 MPa and 4% vertical strain. The DEM result has more obvious fluctuations after yielding, which indicates the dynamic effects due to particle crushing. A similar behavior can also be found in Lobo-Guerrero and Vallejo (2005) and Fu et al. (2017).

4.1 Particle crushing patterns

Fig. 7 illustrates the simulated sand sample at different vertical strains. It is seen that with the increasing vertical strain, more and more particles experienced crushing. Most fragments are found to stay in the vicinity of the original particle location but some may migrate to surrounding voids after further deformation. Fig. 8 compares the 3D views of crushed particles from the simulation and the experiment. It is interesting to see a very good agreement existing between the sequence and locations of major particle crushing events occurring in the simulation and in the experiment, although there is still a difference in the detailed crushing patterns. The fragments generated by the same particle crushing event are labeled in the same color. Note that for the experiment, the corners of the loading board are not right angles, so some fragments can move outside the sample. Three typical examples of crushed particles replaced by fragments are shown in Fig. 9. It is seen that the particles whose maximum contact forces satisfy the particle breakage criterion are represented by a convex hull colored in blue. A number of fragments which are selected from a specific template according to the outputted axial strain are created within the convex hull, and will be used to

replace the crushed particles. The size of the generated fragments follows the AG/SAG breakage probability model.

Fig. 10 shows the evolutions of the mass loss ratio (MLR) and the total number of particles with the increasing vertical strain. A very good model prediction of the total number of particles matching the experimental result is seen, especially within the strain range of 0% - 7%. The total number of particles increases to about 1,300 at the end of simulation, which is more than four times the number of particles at the initial state. The MLR is the ratio of the difference between the current sample mass and the initial sample mass to the initial sample mass. It is found that the entire curve of the MLR exhibits a roughly bilinear pattern, with the rate of increase of mass loss ratio increasing considerably after about 4% strain, which corresponds to the yielding point of the sample (Fig. 6). This behavior is reasonable since significant particle breakage occurs after the yielding point and leads to the continuous accumulation of mass loss. The final MLR reaches 4.99% at the end of the simulation, which is not very significant and does not adversely affect the model performance. It is interesting to note that the final MLR is almost equal to the final value of volume loss of the crushed LBS particles that were reassembled by the authors (Wu and Wang (2018, 2019); Wang and Wu (2020)) using the advanced image matching techniques. This observation reconfirms the minor role of the fine particles in the macroscopic mechanical behavior of granular soils.

4.2 Specific surface area and fractal dimension

The specific surface area is an important parameter for measuring the particle breakage degree and is calculated by dividing the total surface area of all the particles by the total mass of the specimen (Russell 2011; Wang and Yan 2012). The evolution of the specific surface area with increasing vertical stress is shown in Fig. 11(a). A distinct bilinear pattern is seen. The turning point of the bilinear curve is at about 10

MPa corresponding again to the yielding point of the sample. During the stress range of 0–10 MPa, the specific surface area from the simulation is consistent with the experimental result because few particles crushed at this stage. During the stress range of 10–30 MPa, the specific surface area from the simulation is slightly above that of the experiment, indicating that the statistical fragmentation scheme slightly overpredicts the actual amount of particle breakage. This difference, however, is reduced at the end of the simulation. Fig. 11(b) shows the evolution of the fractal dimension of particle volume with increasing vertical stress. The fractal dimension characterizes the fractal nature of the surface textures of real sand particles, and is obtained from measuring a property with a regular shape but different characteristic size (Ersahin et al. 2006). Contrary to the specific surface area, it is seen that the model prediction of the fractal dimension is in good agreement with the experimental result using the AG/SAG breakage probability model.

4.3 Coordination number

The comparison of CN distributions is shown in Fig. 12. The evolution of CN distribution curves from the experiment and simulation exhibits three main features: 1) the initial frequency distributions of CN from both the experiment and simulation show a single peak at $CN = 6$, suggesting a dense packing state close to the hexagonal packing for a narrowly graded granular material; 2) the major peak of the curve shifts towards the left during shearing and tends to be decomposed into 2 subpeaks at larger strains (strain > 7%); 3) the magnitude of the major peak decreases moderately and such a reduction is compensated by an increase of the second subpeak at $CN = 1 \sim 3$.

It is noted that a typical discrete fragmentation method requires to consider the following three aspects of the particle crushing pattern: fragment size distribution, variation of fragment shape and spatial distribution of fragments. Because the complete

determination of this information of every single piece of fragment of real sand particles is basically mission impossible, a feasible and viable approach is to acquire the statistical distributions of these parameters from a representative assembly of sand particles. Such an approach has been adopted for the determination of the first two aspects of the particle crushing pattern.

For the variation of fragment shapes, its statistical feature has been captured by the analysis of CT data and incorporated into the DEM modeling through the generation of 5 virtual fragment templates. For the distribution of fragment sizes, the AG/SAG breakage probability model (Bruchmüller et al. 2011) which computes the breakage index t_{10} was adopted in this study. The third aspect of the particle crushing mode, i.e., the spatial distribution of fragments, however, was not considered in this study. This is because the accurate determination of the positions and orientations of all the fragments requires a powerful image tracking and matching algorithm for crushed sand particles, which is still unavailable at present. Although the authors have achieved some preliminary success in matching a small assembly of crushed sand particles (Wang and Wu 2020; Wu and Wang 2019), implementing the matching algorithm to a specimen of thousands of crushed particles is still impracticable. Therefore, a random distribution of fragments was adopted in this study, which is the reason why the CN result does not match with the experimental data very well. Such a practice has also been adopted by many other authors for investigating the breakage behavior of spherical brittle particles (e.g., Bruchmüller et al. 2011; Zhou et al. 2016; Cil and Buscarnera 2016).

It is worth mentioning that the current fragment replacement modes were only proposed for spherical particles. In these modes, the relative sizes, positions and distribution of fragments are artificially prescribed before the particle crushing event. The direct application of these idealized fragmentation modes to real sand particles is

impracticable.

Therefore, we conclude that the proposed statistical particle fragmentation scheme makes the best use of the CT data for an authentic and accurate modeling of successive particle crushing. However, it is still not possible (and perhaps not necessary) to fully reproduce the exact fragmentation mode of each particle and the post-crushing local fabric change. In fact, there is no unified method for discrete particle fragmentation and therefore, fully reproducing the particle crushing behavior within a loaded assembly of sand particles is still a challenge at the moment. The possible improvement that can be made in the future work includes a refinement on the statistical particle fragmentation scheme to achieve a better reproduction of the local fabric and stress redistribution condition.

4.4 Major contact force chain

A clear advantage of DEM is that the inter-particle contact force data can be easily accessed. This advantage will be taken to facilitate an analysis of MCFC and its SGS within the physical sample. We first plot in Fig. 13 the cumulative probability curve of normalized contact forces within the whole sample (NCF-S) compared with the curve of normalized contact forces that are only carried by fragments (NCF-F) (no matter whether the fragments are in contact with other fragments or intact particles) at different strain levels. The NCF is obtained by dividing the contact force by the average contact force of the whole sample. Clearly, for both cases, the maximum NCF increases with the increasing strain. However, it is interesting to note that more than 65% of NCF-F is equal to or very close to zero; and the maximum NCF-F is always less than 2 and is only about 1/6 of maximum NCF-S at all strain levels. These observations indicate again that the crushed particles play a much less significant role in sustaining the contact force chains within the granular sample.

Next, we extract the MCFC (i.e., contact force $\geq$ average contact force) from the DEM simulation and copy them into the physical sample. The SGS can then be obtained by deleting all the particles that are not involved in the MCFC. A comparison of the SGS from the physical sample and the DEM simulation is shown in Fig. 14. A visual inspection reveals that there is an overall good agreement in the locations and morphologies of particles comprising of the SGS and most of the small fragments are absent from the SGS. A further comparison is made by plotting the particle size and aspect ratio distributions of the two sets of SGS in Fig. 15. It is seen that a very good agreement exists between the two distributions, regardless of the fragmentation degree of the sample. The above results reconfirm that the proposed modeling approach is capable of reproducing, with a high degree of accuracy, the experimental results of the crushing behavior of sands.

4.5 The effects of initial seed generators and steps for breakage check

An additional parametric study to investigate the effects of initial seed generators was performed. The results are shown in Fig. 16. It is seen that using different seeds to initialize the particle strength, the overall stress-strain curve, compressibility and yielding point almost remain unchanged, demonstrating that the modeling results are not sensitive to the seed generator. Another additional parametric study to investigate the effects of steps for breakage check was also conducted. The results are shown in Fig. 17. It is seen that using different steps for breakage check, the stiffness and yielding point almost remain unchanged, demonstrating that the modeling results are not sensitive to this parameter.

4.6 Discussion

Finally, we comment further on the merits and limitations of the proposed approach of modeling realistic particle breakage behavior. Ideally, any particle crushing event should be judged and predicted by a crushing criterion that is an intrinsic function

of the material properties and loading conditions. However, it should be noted that such a perfect particle crushing criterion that can account for not only the onset of crushing, but also the post-crushing events including the exact fragmentation pattern, number, size and shape distributions of all fragments and their contact configurations with the surrounding particles, as well as the associated stress redistribution and energy dissipation behavior, does not exist and whether it can be created in future remains unknown. Under such a circumstance, the current approach of statistical particle fragmentation scheme makes a full use of the CT data of real particle crushing events and uses such information to instruct the DEM model to predict particle crushing. Such an idea is conceptually innovative, appealing, and promising to open a new avenue towards the more accurate, effective, robust and affordable modeling of the real particle crushing behavior of granular materials.

Nevertheless, this is the first step of this line of research on CT-based statistical DEM modeling of granular soils and many further improvements can be made in our future work to enhance its predictive capability and make it less dependent on the CT test. For example, a large database of different types of real sand particles and their crushed fragments can be established from CT tests in future, linking the particle size and morphological features to the external stress or strain applied to an assembly of such particles. With such a database, it is possible to establish a fully independent and intelligent DEM model that can predict the mechanical behavior of crushable soils on its own.

5 Concluding remarks

In this paper, an innovative study on DEM modeling of successive particle breakage events occurring within a mini sand specimen using a statistical particle fragmentation scheme is conducted. Following the recent work of Wu and Wang (2020)

on the modeling of single particle breakage, this work takes a further step to incorporate the realistic shapes of fragments resulting from particle crushing based on the micro-CT data of particle fragmentation within the mini-specimen subject to 1D compression test. The major contribution of this study lies in the following three aspects: 1) precisely reconstructing the initial specimen based on one-to-one mapping of every sand particle utilizing SH analysis; 2) creating virtual templates of fragments using CT data of crushed particles obtained at different stages of the test; and 3) combining DEM and CT data to make an analysis of MCFC and SGS. Through a comprehensive comparison of the simulation and experimental results, we conclude that the proposed statistical particle fragmentation scheme is capable of reproducing both the macro-scale and particle-scale behavior of the particular sample of 308 grains with a high degree of accuracy.

The proposed approach offers a new idea of modeling realistic particle breakage behavior. Given the fundamental and frontier nature of this work, the prospective application of the proposed method can be envisioned to the scientific research not only in geomechanics but also in many other fields such as granular materials, powder technology, coal mining and petroleum engineering or even meteorology. The following limitations of this work should also be acknowledged: 1) the generation of virtual fragment templates requires the access to CT data, which limits the direct application of the approach to the modeling of other sands or granular materials; 2) the use of the macro state variable (e.g., macroscopic strain or stress attained in 1D compression) to invoke the virtual fragment template for particle replacement may restrict the application of the modeling approach to other stress/strain path or boundary value problems.

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