# **Computers and Geotechnics**

# 3D modelling of soil-rock mixtures considering the morphology and fracture characteristics of breakable blocks --Manuscript Draft--

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Abstract:	Failure mechanisms of a soil-rock mixture (S-RM) can be efficiently investigated by the discrete element method (DEM). This paper proposes a stochastic approach for 3D DEM modelling of S-RM samples accounting for morphological features and internal fractures characteristics of breakable blocks. The research refers to an artificial S-RM filling slope, mainly containing highly-weathered shale blocks, located in the Yunnan Province, China. The 3D morphological features of the blocks and the characteristics of their internal fractures were obtained by CT technology and image processing. A stochastic method based on harmonic series was developed, allowing the generation of random block clusters with characteristics similar to the original ones. Another stochastic approach was implemented for the creation of the internal fractures, simulated as voids in the block clusters, following the characteristic of the real fractures. Finally, the procedure was applied for the definition of a 3D S-RM DEM model with 40% block proportion, whose meso-parameters were determined for simulating direct shear tests. The numerical results showed that the generated random S-RM DEM model well reproduced the experimental behaviour of S-RM samples with breakable blocks. Also, they highlighted the importance of modelling the block breakage and internal fractures by companion simulations.	

Dear editorial board of Computers and Geotechnics,

Please find enclosed the revised manuscript: "3D modelling of soil-rock mixtures considering the morphology and fracture characteristics of breakable blocks", by Han Zhang, et al., for a possible publication as a Research Paper in Computers and Geotechnics. All co-authors cooperated and agreed with the contents of the manuscript. We certify that the submission is an original work and is not under review in any other journals.

We have performed the revisions according to the suggestions by the editors and reviewers, the revised portions are marked in red in the manuscript.

Sincerely yours,

Corresponding author: Han Zhang Faculty of Engineering, China University of Geosciences , Wuhan , 430074, China Email address: zhanghan@cug.edu.cn.

# **Response of Reviewers comments**

We thank the Reviewers for their valuable comments concerning our manuscript. They were all helpful for improving our paper. We studied all comments carefully and made the requested corrections, which we hope will meet their approval. Revised portions are marked in red in the manuscript. The main corrections and the reply to the Reviewers' comments are as follows:

## **Reviewer 1**

**Comment#1:** 1. L13-16 of Page 4. The following relevant papers on X-ray CT characterization of 3D contact fabric and grain kinematics of sands under shear might be worthy of a mention:

[i] Cheng, Z., & Wang, J. (2018). Experimental investigation of inter-particle contact evolution of sheared granular materials using X-ray micro-tomography. Soils and Foundations, 58(6), 1492-1510.

[ii] Cheng, Z., & Wang, J. (2018). A particle-tracking method for experimental investigation of kinematics of sand particles under triaxial compression. Powder Technology, 328, 436-451. **Response#1:** 

Thanks for your recommendation: these relevant papers were introduced in Section 1.

**Comment#2:** L18-20 of Page 4. 'However, the exact one-to-one mapping of the CT images into the corresponding model is clearly an unfeasible choice ...' It may be worthwhile to refer to the following work on DEM modeling of sand based on one-to-one mapping of CT images:

[iii] Wu M., et al. (2020). DEM modelling of mini-triaxial test based on one-to-one mapping of sand particles. Géotechnique, 1-14.

## **Response#2:**

We referred to this paper in Section 1 as follows:

The exact one-to-one mapping of the CT images were used to establish a DEM model of a mini-triaxial sand specimen 8 mm in diameter and 16 mm in heigth (Wu et al., 2020). However, this approach cannot be followed at the moment for modelling large-scale samples, as the S-RM ones used in the discussed in-situ tests.

**Comment#3:** I think there is a mistake in Line 6 of Page 6. Referring to Fig. 2a, diameter is 145 mm and height is 285 mm?

## **Response#3:**

Yes, the text was corrected into "The pipes, labelled as C1, C2 and C3 (Fig. 2a), had a diameter of 145mm and a height of 285mm.".

**Comment#4:** Line 13-14 of Page 6. Does the 3D CT image have a voxel size of 0.45 mm×0.45 mm×0.6 mm? I think it is better to use' voxel size' instead of 'pixel size' here.

## **Response#4:**

Yes, the voxel size of a 3D CT image is  $0.45 \text{ mm} \times 0.45 \text{ mm} \times 0.6 \text{ mm}$ . We agree with the reviewer that the use of "voxel size" is more accurate than "pixel size" and we revised the manuscript accordingly.

**Comment#5:** Fig. 3a- Referring to your median filter size, I guess your image processing is implemented on 3D images. Am I right? It should be clarified in the text.

## **Response#5:**

Yes, the image processing was performed on the 3D CT images, referring not only to the median filter but also to the 26-neighborhood connected components extraction and watershed-based separation. This point was clarified it in the revised manuscript.

**Comment#6:** Figs. 10b & 10c suggest that  $S_p$  and R are scale-dependent, i.e., the accuracy of  $S_p$  and R are dependent on the grain size. The reason should be explained in the text.

## **Response#6:**

Figure 10c & 10d reveals that  $S_p$  and R are more difficult to be described, necessitating a higher value of n, especially for the blocks with the larger particle size. This is because these larger blocks are characterised by a larger angularity and more complex morphological details (see Figure 4c), indicating the description of the block surface with larger size needs more harmonics series than the smaller one. This explanation was added to the text following the reviewer's suggestion.

**Comment#7:** Fig. 7b What does  $N_f$  in the y axis represent? Should it be  $F_f$ ? Does  $F_f$  of Eqs. 7, 10 and 11 refer to the same thing, i.e., fracture number? It should be mentioned in Eq.7 that the calculation based on this equation could lead to non-integer values.

## **Response#7:**

We thank the reviewer for having found this mistake that we promptly corrected. In fact, in the Fig. 7b, the label of *y* axis is  $F_f$  instead of  $N_f$ . The  $F_f$  in the Eqs. (7), (10) and (11) all refer to fracture frequency. It was mentioned in the text: the  $F_f$  calculated by Eqs. (7), (10) and (11) maybe non-integer values.

**Comment#8:** The number of '5.2' of Fig. 5a is not consistent with '5.3' in Eq. 7.

## **Response#8:**

Again, we thank the reviewer for his careful correction. Yes, the mean value of the Gaussian function in Eq. 7 is 5.2, as shown in Fig. 5a.

Comment#9: Line 24 of Page 18. The version of the particle flow code software should also be specified.

## **Response#9:**

The version of the particle flow code used in the simulation of the soil-rock mixtures is  $PFC^{3D}5.0$ , now specified in the revised manuscript.

**Comment#10:** Line 9 of Page 19. 'The maximum fracture size is 0.8 mm'? Please verify whether this is correct.

## **Response#10:**

We corrected the text into "The minimum fracture size is 0.8 mm".

**Comment#11:**Page 24 of Section 4. The soils with a grain size range of 4.8-5.0 mm were generated in the DEM model. It seems that the realistic morphologies were not considered in the DEM modeling for soil grains, while those were modelled for the blocks. Why? The reasons should be mentioned in the paper.

## **Response#11:**

In our study, the soil particles were simplified as sphere balls in the S-RM DEM models, similarly to other DEM studies of S-RM (e.g. Xu et al., 2016b). This simplification is mainly due to the limited computation capacity. Although the morphology of soil particles can be represented by bonding several smaller balls, this will lead to a large increase in the particle number in the DEM model. As such, the irregular morphology of soil particles was neglected and the rolling resistant model was adopted for simulating their roughness (Jiang et al. 2005, Xu et al. 2016b).

**Comment#12:** The paper needs to be carefully proofread to eliminate all typos and grammar errors. See for example:

Line 22 of Page 5: 'wan' should be 'was'?

Line 11 of Page 15: 'serious' should be 'series'

Line 2 of Page 18: 'fuction' should be 'function'.

Line 11 of Page 18: 'Similarly' should be 'Similar'

## **Response#12:**

We thank the reviewer for these careful checks. Spelling mistakes were corrected and the text was checked again.

# **Reviewer 2**

**Comment2#1:** Eqs. (3) and (6) are purely empirical and dimensional consistency is not satisfied. Therefore, the unit of D in this equation should be clarified.

## Response2#1:

The unit of the particle size of blocks D in Eqs. (3) and (6) is in mm. The revised manuscript was corrected accordingly.

**Comment2#2:** Explanation to the observed relative orientation distributions of fractures, as shown in Fig. 7, should be given.

## Response2#2:

The  $\theta$  values mainly lie in the ranges 0 ° - 40 ° and 120 ° - 180 °, while  $\gamma$  in the 30 ° - 70 ° one. This is because the inter-fractures commonly formed along the stratification orientation of the shale blocks under the compaction stage during the slope filling.

**Comment2#3:** In the DEM analyses, soil particles are modelled as balls and irregular morphology of the particles is not taken into account. Limitation of the assumption should be addressed.

## Response2#3:

The limitation was mentioned in the text:

Considering of the limitation of the computation capacity, the soil particles in the DEM model were simplified as spherical balls having radii from 4.8 mm to 5.0 mm. Although the morphology of soil particles can be represented by bonding several smaller balls, this will lead to a large increase in the particle number in the DEM model. As such, the irregular morphology of soil particles was neglected and the rolling resistant model was adopted for simulating their roughness (Jiang et al. 2005, Xu et al. 2016b).

# Highlights

- 1. A stochastic generation approach, accounting for the morphological features and internal fractures characteristics of breakable blocks, was proposed and applied to the 3D DEM modelling of S-RM.
- 2. A stochastic method was developed for generating random blocks with characteristics similar to the real ones on the basis of spherical harmonic series.
- 3. A stochastic approach was proposed for creating random fractures on the basis of the characteristics of the real ones.
- 4. It was demonstrated that neglecting block breakage and the presence of internal fractures had significant influence on the shear strength of the S-RM sample by companion simulations.

1	3D modelling of soil-rock mixtures considering the morphology and
2	fracture characteristics of breakable blocks
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## 1 ABSTRACT

Failure mechanisms of a soil-rock mixture (S-RM) can be efficiently investigated by the discrete element 2 method (DEM). This paper proposes a stochastic approach for 3D DEM modelling of S-RM samples 3 accounting for morphological features and internal fractures of blocks and their potential breakage. The 4 research refers to the case-history of an artificial S-RM filling slope, mainly containing highly-weathered 5 6 shale blocks, constructed at the ±500kV electronic converter station in the Funing County, Yunnan Province, China. The 3D morphological features of the blocks and the characteristics of their internal 7 fractures were obtained by CT technology and image processing. A stochastic method based on harmonic 8 series was developed starting from the real blocks, allowing the generation of random block clusters with 9 10 characteristics similar to the original ones. Another stochastic approach was implemented for the creation of the internal fractures, simulated as voids in the block clusters, following the characteristic of the real 11 12 fractures. Finally, the procedure was applied for the definition of a 3D S-RM DEM model with 40% block proportion, whose meso-parameters were determined for simulating direct shear tests. These latters 13 were also useful to explore the mechanical response of the sample at the meso-scale, including the 14 formation and development of the localization band. The numerical results showed that the generated 15 random S-RM DEM model well reproduced the experimental behaviour of S-RM samples with breakable 16 blocks. Also, they highlighted the importance of modelling the block breakage and internal fractures; in 17 18 fact, companion simulations with unbreakable blocks and breakable blocks without fractures were all characterised by increased shear strength with higher friction angle but reduced cohesion. 19

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- 21 22
- Key words: soil-rock mixture; random block generation; random fracture generation; 3D S-RM DEM model; mechanical behaviour of S-RM
- 25

## 1 **1. Introduction**

Soil-rock mixtures (S-RMs) were defined by Xu (2008) as extremely inhomogeneous geomaterials 2 composed of rock blocks, with various sizes and a relative high strength, and a fine-grained soil matrix. 3 The rock-matrix interface is unbounded in the S-RMs, in contrast to bimrocks (Medley, 1994). S-RMs are 4 widespread in natural landslides (Sonmez, 2006; Xu et al., 2007; Yang et al., 2019) but are also 5 commonly used as filling materials in embankments and artificial slopes (Calseira & Brito, 2014; Zhang 6 et al., 2016; Cen et al., 2017). To assess the stability of such geo-structures, several researches have 7 investigated their mechanical properties by laboratory (Dong, 2007; Hamidi et al., 2011; Liu et al., 2017) 8 9 and in-situ (Xu et al., 2011; Coli et al., 2011; Zhang et al., 2016; Zhang et al., 2020) tests. The experimental evidence has shown that the mechanical properties of S-RMs are not only controlled by the 10 volumetric block proportion (VBP), but also by block shape and strength, this latter affected by the 11 potential presence of pre-existing internal fractures. However, the analysis of all the complex failure 12 13 mechanisms occurring during the experiments, including those controlled by the shape and strength of the rock blocks, is practically unfeasible. 14

Numerical modelling, and especially the discrete element method (DEM) approach, is undoubtedly a powerful tool for revealing the failure mechanisms in S-RMs. However, accuracy of calculations is strictly connected to the capacity of the numerical model to reasonably account for the peculiar characteristics of these materials, including those related to the shape of the rock blocks and to the possible presence of pre-existing fractures.

Nowadays, 2D numerical S-RM models are mainly generated following two possible strategies, the first 20 21 one making use of stochastic algorithms (Li et al. 2004; Xu et al., 2016a; Chen et al., 2018) and the other one based on digital image processing (DIP) (Yue et al., 2003; Xu et al., 2008; Hu et al., 2018). Li et al. 22 (2004) created S-RM stochastic numerical models using the Monte Carlo random sampling principle, the 23 spatial distribution and size distribution of rock blocks obeying an even and a normal distribution law, 24 25 respectively. A multi-circle block generation method, adopted for the subsequent generation of 2D DEM S-RM models, was developed by Xu et al. (2016a) considering the size distribution and spatial location of 26 rock blocks. Chen et al. (2018) proposed an aggregate structure generation method based on an enhanced 27 procedure of random sequential addition, significantly reducing the computational cost, and established 28 29 S-RM models with a high VBP. In all these stochastic S-RM models, the shape of rock blocks is that of 30 simple convex polygons, ignoring their real morphology. In order to overcome this limitation, Yue et al.

(2003) used digital image processing (DIP) for generating 2D FEM models in which rock blocks with real
shapes were derived from 2D images. The DIP technique was also employed in the set-up of 2D DEM
models of S-RMs by Xu et al. (2008) and Hu et al. (2018).

3D numerical models, more representative of the real structure of S-RMs and bimrocks, have been also 4 recently developed. Cheng et al. (2010) created 3D S-RM DEM models with different VBP on the basis 5 of the particle bonding method, the blocks deriving from the bonding of a group of elementary spheres. 6 7 Coli et al. (2012) proposed 3D FEM bimrock models containing different ellipsoidal (e.g. prolate, sphere and oblate) rock blocks for the simulation of uniaxial and triaxial compression tests. Xu et al. (2016b) 8 9 developed 3D random systems and established 3D DEM S-RM models, with no overlap between two bonded spheres in a convex polyhedron rock block clump, for the analysis of failure mechanisms of 10 S-RMs during direct shear tests. Nevertheless, the shape of rock blocks in these 3D numerical models is 11 also limited to that of simple polyhedrons. 12

The X-ray computed tomography (CT) technology has been widely used for the 3D visualization and 13 14 characterisation of the shape and structure of geomaterials (e.g. Masad et al., 2005; Fonseca et al., 2012; Zhao et al., 2015), generating 3D numerical models of sand assembly (Zhou et al., 2016; Zhou & Wang, 15 2017; Xu et al., 2020), and investigating the movement and contact evoluation characteristics of sand 16 17 particles in the shear process under the triaxial compression (Cheng & Wang, 2018a; b). Some features of rock fractures, such dimension, roughness and spatial distribution were investigated using CT images by 18 19 Kolyukhin et al. (2014) and Liang et al. (2016). The exact one-to-one mapping of the CT images were used to establish a DEM model of a mini-triaxial sand specimen 8 mm in diameter and 16 mm in height 20 21 (Wu et al., 2020). However, this approach cannot be followed at the moment for modelling large-scale samples, as the S-RM ones used in the discussed in-situ tests. Relatively few researches have established 22 reasonable stochastic approaches for the definition of rock block models considering real 3D multi-scale 23 morophological features, such as the roundness in addition to dimension and sphericity. Furthermore, the 24 internal structure of rock blocks, related to the presence of fractures and voids, has still never been 25 accounted for. 26

This study proposes an experimental-mathematical approach for the generation of 3D DEM S-RM models accounting for block morphology and characteristics of block internal fractures. The research refers to the case-history of an artificial S-RM filling slope constructed at the ±500kV electronic converter station in the Funing County, Yunnan Province, China. The filling material adopted at the site mainly consisted in a

sandy silt matrix and highly-weathered shale blocks. For an economic and safe design, some large-scale 1 direct shear tests were performed for assessing the shear strength properties of the S-RMs. After testing, a 2 limited number (e.g. 300) of shale blocks of different sizes (10 - 80 mm) were scanned and reconstructed, 3 on the basis of CT technology and image processing, for obtaining their morphological features and the 4 characteristics of their internal fractures. Stochastic methods were developed, using SH series and 5 characteristic distributions of real blocks and fractures, for establishing random blocks and fractures with 6 7 characteristics similar with the real ones. DEM models were then implemented simulating the blocks as clusters and the fractures as voids. In particular, a S-RM DEM model with 40% VBP was considered to 8 9 analyse the mechanical response of the material during direct shear tests.

10

## 11 **2.** Morphological characteristics of the shale blocks and of their internal fractures

12 2.1 3D CT reconstruction of shale blocks

13 2.1.1 Shale blocks in the S-RM samples

The considered S-RM is mainly composed of sandy silt matrix and highly-weathered shale blocks, as shown in Fig. 1a. The shale blocks are made of 76.15% of quartz and 23.85% of chlorite, with average values of dry density  $\rho_d = 1.577$  g/cm<sup>3</sup>, particle weight  $G_S = 2.902$ , porosity n = 36.5 % and unconfined compressive strength UCS = 4.3±1.5 MPa (Zhang et al., 2020).

During the construction of the electronic converter station, one of the artificial slopes experienced large 18 lateral displacements due to the overestimation of the shear strength of the S-RM at the design stage. As 19 20 such, some large-scale direct shear tests (DST) were performed with a cylindrical shear box 400 mm in height and 560 mm in diameter (Fig. 1b). The threshold particle diameter  $d_{thr}$ , formally separating the 21 matrix from the blocks, was defined following Medly (1994) as  $d_{thr} = 0.05 L_c$ , where  $L_c$  is the 22 characteristic engineering scale. Specifically,  $L_c$  was taken equal to the apparatus half height, equal to 200 23 mm, providing a threshold value of 10 mm. The maximum particle size of the blocks, collected from the 24 artificial slope, was not larger than 80 mm, corresponding to 1/5 of the semi-height of shear box. The 25 tested S-RM samples were characterised by a VBP of 35% - 60%. 26



(a) Shale blocks in the S-RM(b) large-scale direct shear apparatusFig. 1 Shale blocks employed in the artificial slope and the large-scale direct shear apparatus

## 2

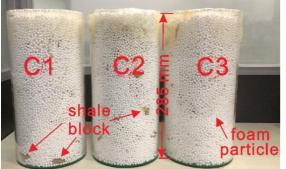
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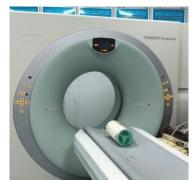
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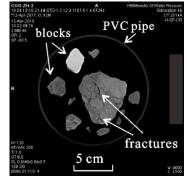
## 3 2.1.2 3D CT reconstruction

CT technique was applied to reconstruct the 3D morphology of the blocks and the main features of the 4 fractures. About 250 undisturbed (i.e. not affected by the failure process) shale blocks ranging from 10 5 6 mm to 80 mm were randomly picked from the S-RM samples after the DSTs and placed into three PVC pipes for CT scanning. The pipes, labelled as C1, C2 and C3 (Fig. 2a), had a diameter of 145mm and a 7 height of 285mm. Foam particles of very low density were adopted to fill the pipes and isolate the blocks. 8 The Siemens Somatom Sensation 40 CT system (Fig. 2b), provided by the Key Laboratory of 9 Geotechnical Mechanics and Engineering of the Ministry of Water Resources, Yangtze River Scientific 10 Research Institute, was employed to perform the X-ray CT scanning and acquire a series CT images. As 11 shown in the CT image of Fig. 2c, the blocks and their internal fractures were clearly observed. Each of 12 13 these images consisted of 512 voxels by 512 voxels, with a resolution of 0.45 mm/voxel and a thickness

of 0.6 mm. The voxel size of the 3D CT image is  $0.45 \text{ mm} \times 0.45 \text{ mm} \times 0.6 \text{ mm}$ .







(a) CT samples of shale blocks (b) CT system Fig. 2 Image acquisition using X-ray CT technology

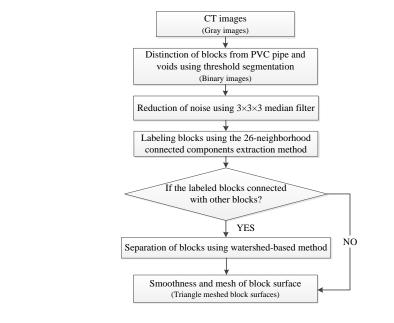
(c) CT tomographic image

16 The individual blocks and the fractures were extracted from the CT images by following a series of

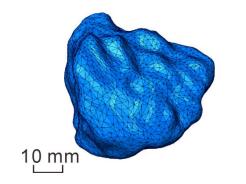
processing steps, consisting in segmenting the different portions, reducing the noise, separating and labelling individual objects, as summarised in Fig. 3a. The image processing was implemented on 3D images, referring not only to the median filter but also to the 26-neighborhood connected components extraction and watershed-based separation. The triangle meshed surfaces of one block is shown in the Fig. 3b.

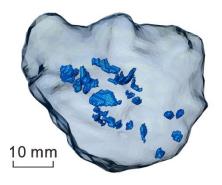
6 The CT images of the fractures were obtained by inverting the binary CT images and removing the 7 connected component representing the background, characterised by the highest number of voxels. Then, 8 the surfaces of internal fractures in a block were reconstructed (Fig. 3c) by performing the same image 9 process.





(a) Flowchart of image processing of CT reconstruction





(b) 3D morphological reconstruction of block

(c) 3D morphological reconstruction of fractures

Fig.3 Image processing and 3D CT reconstruction of block and fracture surfaces

11

12

1 2.2 3D morphological features of the shale blocks

The morphological features of particles can be described, from the largest to the smallest scale, in terms
of form, roundness and surface texture (Barrett, 1980; ISO, 2008). The particle form is typically assessed
in terms of principal dimensions (and related elongation and flatness) and sphericity (Zheng & Hryciw,
2015). They are defined as described in the following.

6 (1) Elongation and Flatness

7 The 3D principal dimensions, named long  $l_a$ , intermediate  $l_b$  and short  $l_c$  axis dimension, can be obtained by the so-called principal component analysis of the particle vertices (Fu et al., 2018). In this paper, the 8 9 principle intermediate dimension  $l_b$  was considered as the block particle size D. The block principal 10 dimensions were used to assess the block form by two widely used descriptors: the elongation index (EI) and the flatness index (FI), with  $EI = l_b / l_a$  and  $FI = l_c / l_b$ . The block form was commonly defined according 11 to the four categories: spheroid (if EI > 2/3 and FI > 2/3), oblate (if EI > 2/3 and FI < 2/3), prolate (if EI < 1/3) 12 2/3 and FI > 2/3), and blade (if EI < 2/3 and FI < 2/3). As shown in Fig. 4a, the shale blocks considered in 13 14 this study are mainly spheroidal and oblate, with only few prolate and blade. Their EI index is in the range 0.5 to 1.0, while the corresponding FI values vary from 0.4 to 1.0. The principle dimensions of the 15 blocks were found to obey the following rules: 16

17 
$$\begin{cases} D \le l_a \le 2D\\ 0.4D \le l_c \le D \end{cases}$$
(1)

18 (2) Sphericity

Sphericity  $(S_p)$  can be used for evaluating how much a block resembles a sphere. It is defined as the ratio of the surface area of a sphere, having same volume V of the block particle, to the actual block surface area S:

$$S_p = \frac{\sqrt[3]{36\pi V^2}}{S} \tag{2}$$

The sphericity  $S_p$  of blocks are in the range of 0.7 - 0.97, with smaller values for larger D (Fig. 4b), indicating that smaller blocks are more similar to a sphere than the larger ones. The two quantities  $S_p$  and D are always bounded by two lines having the following equations:

$$-0.0006 D + 0.730 \le S_p \le -0.0014 D + 0.984$$
(3)

27 where the unit of D is mm.

## 1 (3) Roundness

Roundness is a descriptor representing the particle angularity (Wadell, 1932), being blocks with smaller roundness those having higher angularity. The 3D roundness was calculated in previous researches (Bullard & Garboczi, 2013; Zhou et al., 2017) by the maximum curvatures  $\kappa_{max}$  of particle surface vertices. The  $\kappa_{max}$  of a vertex of the block surface can be calculated on the basis of Gaussian curvature and mean curvature; the corresponding minimum curvature radius  $r_{min}=|\kappa_{max}|^{-1}$  can be used to estimate whether a vertex on the block surface is a 'corner':

$$g(\kappa) = \begin{cases} 1 & \text{if } r_{min} < r_{ins} \\ 0 & \text{if } r_{max} \ge r_{ins} \end{cases}$$
(4)

9 The function g, called corner judgment function, is equal to 1 or 0 if the vertex is a 'corner' or not, 10 respectively, and  $r_{ins}$  is the radius of the maximum inscribed sphere of the block particle. The 3D 11 roundness R of the block particle is then obtained as:

12 
$$R = \frac{\sum_{i=1}^{N} g_i(\kappa) r_{min}^i}{Nr_{ins}}$$
(5)

n

where  $g_i(\kappa)$  and  $r_{min}^i$  represent the corner judgment and the minimum curvature radius of the *i*th vertex on the block surface, respectively. *n* and *N* are the number of vertices and corners on the block surface, respectively.

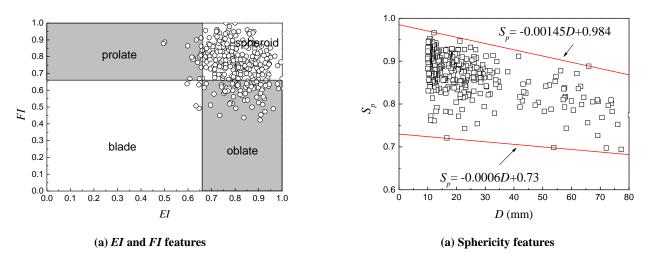
As shown in Fig. 4c, shale blocks with larger particle size have also larger angularity. The 3D roundness R of blocks varies from 0.3 to 0.8, and the values of R and D lie in the range:

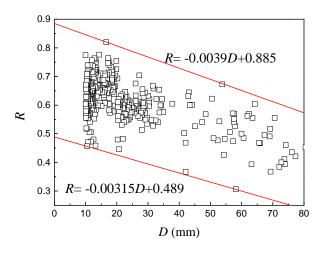
18

8

$$-0.00315D + 0.489 \le R \le -0.0039D + 0.885 \tag{6}$$

19 where the unit of D is mm.

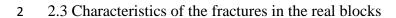




(c) Roundness features Fig. 4 3D morphlogical features of real shale blocks



20



3 (1) Fracture frequency

4 The fracture frequency F corresponds to the number of fractures in each block,  $N_f$ , per unit block volume

5  $V. N_f$  was obtained by the CT reconstructed real fractures: no fractures were found in the blocks with size

6 D less than 40 mm, while  $N_f$  varies from 0 to 31 in the larger blocks with a D value ranging from 40 to 80

7 mm. In general, the average fracture frequency is 0.1 for  $1 \text{ cm}^3$ .

8 (2) Size distribution of fractures

9 The 3D principal dimensions of fractures, indicated respectively with the symbols  $l_{fa}$   $l_{fb}$  and  $l_{fc}$  for the long, 10 intermediate and short dimensions were obtained by employing the principal component analysis of the 11 fracture vertices.

12  $l_{fa}$  values distribute from 2 mm to 16 mm, well obeying to an Amplitude Gaussian distribution with  $l_{fa} \sim$ 13  $y_0+A \cdot N(\mu, \sigma^2)$ , where  $y_0$  and A are the offset and amplitude, and  $N(\mu, \sigma^2)$  is a Gaussian function with 14 mean  $\mu$  and standard deviation  $\sigma$ . The distribution of fracture frequency  $F_f$  with  $l_{fa}$  values can be expressed 15 by:

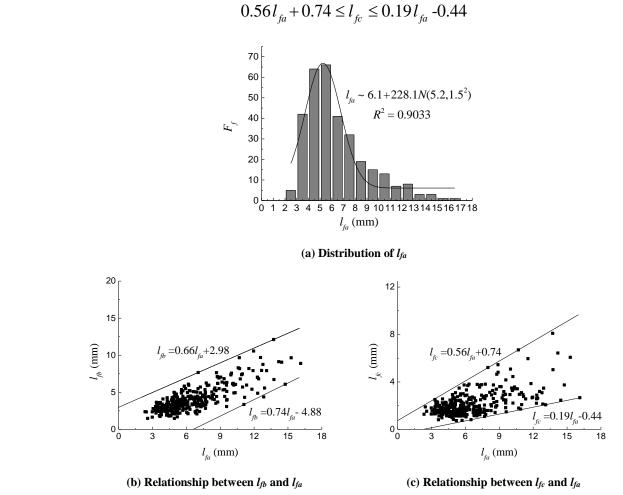
16 
$$F_f = 6.1 + 228.1 N (5.2, 1.5^2) = 6.1 + 228.1 \cdot \frac{1}{\sqrt{2\pi \cdot 1.5}} e^{-\frac{(l_a - 5.2)}{2 \cdot 1.5^2}}, 2 \text{ mm} \le l_a \le 16 \text{ mm}$$
 (7)

Values of  $l_{fb}$  and  $l_{fc}$  are respectively in the range of 1.5 - 12 mm and 0.8 - 8 mm. It is evident that the larger the dimension  $l_{fa}$ , the larger the dimensions  $l_{fb}$  and  $l_{fc}$  (Fig. 5b and 5c). In fact,  $l_{fb}$  and  $l_{fc}$  are bounded by the following expressions:

$$0.74l_{fa} - 4.88 \le l_{fb} \le 0.66l_{fa} + 2.98 \tag{8}$$



2 3



(9)

Fig. 5 3D Size distributions of fractures

4 5

(3) Distribution of fracture relative orientations

6 The relative orientation of a fracture in the block is defined in Fig. 6, where the *x*, *y* and *z* axes are the 7 short, intermediate and long axes of a block, respectively, and the  $z_c$  axis is the long axis of the internal 8 fracture.  $\theta$  is the relative angle between the long axis of block and that of fracture, while  $\gamma$  is the angle 9 between the projection of  $z_c$  on the *xy* plane and intermediate axis of block. They are both defined in the 10 interval [0°, 180°].

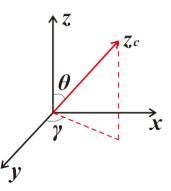




Fig. 6 Schematic of fracture relative orientations in blocks

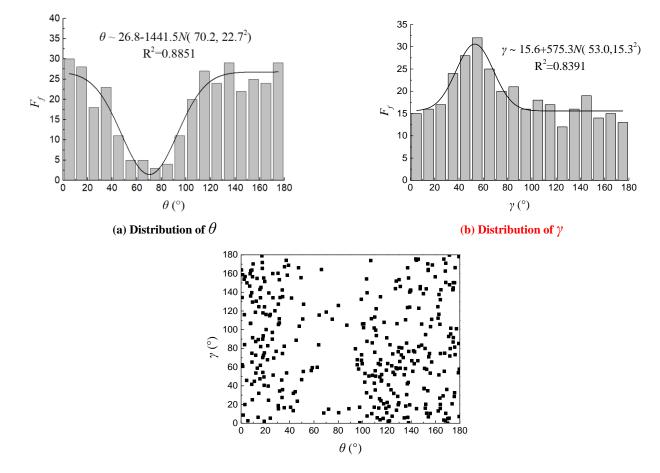
1 The relative orientations of fractures and their distribution features are shown in Fig. 7a and 7b. The  $\theta$ 2 values mainly lie in the ranges 0 ° - 40 ° and 120 ° - 180 °, while  $\gamma$  in the 30 ° - 70 ° one. This is because 3 the inter-fractures commonly formed along the stratification orientation of the shale blocks under the 4 compaction stage during the slope filling. Inspection of Figure 7c reveals that no relationship exists 5 between  $\theta$  and  $\gamma$ . The distributions of fracture orientations are also found to obey Amplitude Gaussian 6 distributions with Eq. (10) and Eq. (11). The fracture frequency  $F_f$  calculated by the Eqs. (7), (10) or (11) 7 maybe non-integer values.

$$F_f = 26.8 - 1441.5 \bullet \frac{1}{\sqrt{2\pi} \bullet 22.7} e^{\frac{(\theta - 70.2)^2}{2 \bullet 22.7^2}} , \quad 0^\circ \le \theta \le 180^\circ$$
(10)

$$F_{f} = 15.6 + 575.3 \bullet \frac{1}{\sqrt{2\pi} \bullet 15.3} e^{-\frac{(\gamma - 53.0)^{2}}{2 \bullet 15.3^{2}}} , \quad 0^{\circ} \le \gamma \le 180^{\circ}$$
(11)

10

9

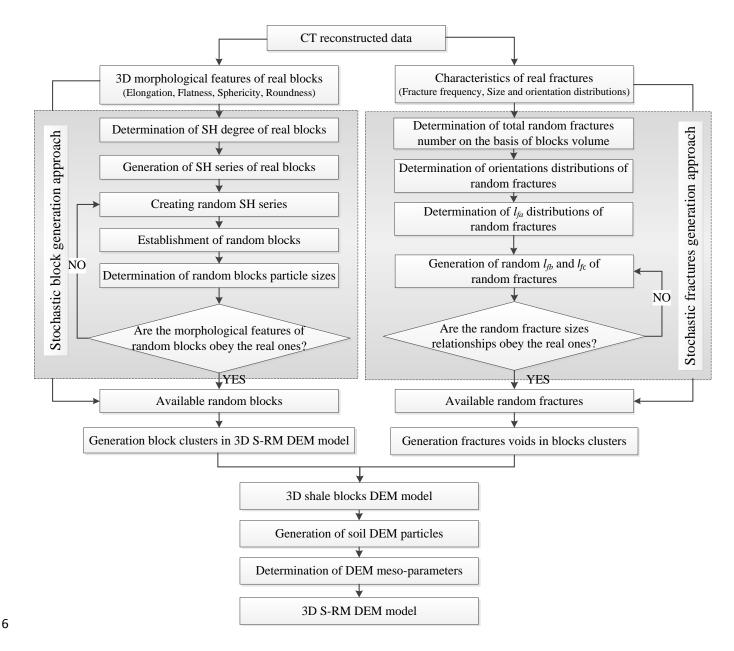


(c) Relationship between fractures relative orientations Fig. 7 Relative orientation distributions of fractures

- 11 12
- 13

## **3.** Generation approaches of 3D random block and fracture models

Due to the large number of rock blocks in the S-RM samples tested in the laboratory, their single scanning was practically unfeasibile. In order to overcome this limitation, block and fracture stochastic generation approaches were proposed, respectively based on spherical harmonics (SH) series of the real blocks and characteristics of the real fractures, and applied to the generation of S-RM DEM models (Fig. 8).



- Fig. 8 Flowchart of generation approach of 3D DEM modelling of S-RM samples
- 8 3.1 Stochastic block generation approach
- 9 3.1.1 Spherical harmonic series of blocks
- 10 The spherical harmonic (SH) series were used in the past to represent and quantify the shape of

aggregates, rock blocks and sand particles on the basis of 3D CT data (Garboczi, 2002; Masad et al., 2005;
 Zhou et al., 2015, 2017; Su & Yan, 2018; Feng et al., 2020). Correspondingly, a new block particle can be
 constructed if a set of spherical harmonic series are created.

The goal of a SH analysis is to expand the polar radius from a unit sphere to the particle surface. The SH
series can be expressed as:

$$r(\theta,\phi) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} a_n^m Y_n^m(\theta,\phi)$$
(12)

7 where  $r(\theta, \phi)$  is the polar radius from the particle centre to its surface vertices  $(0 \le \theta \le \pi, 0 \le \phi \le 2\pi)$  and 8  $a_n^m$  are the associated SH coefficients.  $Y_n^m(\theta, \phi)$  is the SH function given by:

9 
$$Y_n^m(\theta,\varphi) = \sqrt{\frac{(2n+1)(n-m)!}{4\pi(n+m)!}} P_n^m(\cos\theta) e^{im\varphi}$$
(13)

10  $P_n^{n}(x)$  is the associated Legendre function expressed as:

11 
$$P_n^m(x) = \frac{(-1)^m}{2^n n!} (1 - x^2)^{m/2} \frac{d^{n+m}}{dx^{n+m}} (x^2 - 1)^n$$
(14)

where *n* and *m* are the SH degree and order of  $P_n^m(x)$ . Note that *n* is a non-negative integer from zero to infinity according to the required fitting precision, while *m* is the integer from *-n* to *n* so that the total number of a series of  $a_n^m$  is  $(n + 1)^2$ .

15 3.1.2 Determination of SH degree of blocks

As shown in Fig. 9, the morphological features of blocks constructed by the SH series depend on the SH degree n, having the block with higher n an increasing level of resemblance to the CT one. In order to ensure that the morphological features of the SH reconstructed blocks are sufficiently similar with those of real ones, the value of n was fixed reasonably, as discussed in the following.

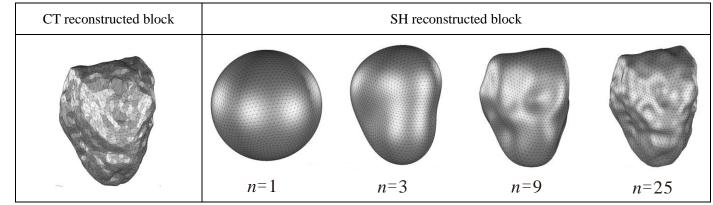




Fig. 9 View of CT reconstructed block and SH reconstructed ones with different SH degrees

Four CT reconstructed blocks, labelled as R1, R2, R3 and R4, with particle size of 75 mm, 41 mm, 28 mm and 14 mm respectively, were selected for assessing the optimum value of *n*. The relative error  $E_{EI}$  in the *EI* values of the SH reconstructed blocks to that of the CT ones is defined as:

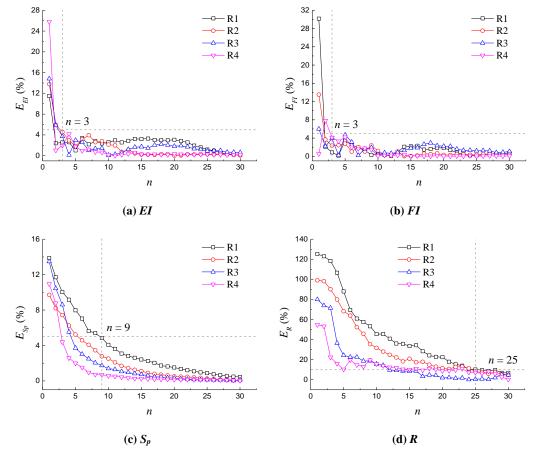
$$E_{EI} = \frac{\left|EI_{SH} - EI_{CT}\right|}{EI_{CT}} \times 100\% \tag{1}$$

5)

5 where *EI*<sub>SH</sub> and *EI*<sub>CT</sub> are the *EI* of the SH reconstructed block and that of the CT one, respectively.

4

6 Similarly, relative errors for *FI*,  $S_p$  and *R* of the SH reconstructed blocks, named respectively as  $E_{FI}$ ,  $E_{Sp}$ 7 and  $E_R$ , can also be defined.



8 Fig. 10 Relationship between valued of n and relative errors of the morphological features of the SH reconstructed blocks As shown in Fig. 10, the EI and FI of blocks reach a stable value for n values higher than 3, with  $E_{EI}$  and 9 10  $E_{FI}$  values both less than 5 %. Inspection of the figure reveals that  $S_p$  and R are more difficult to be described, necessitating a higher value of n, especially for blocks with the larger particle size. This is 11 because these larger blocks are characterised by a larger angularity and more complex morphological 12 details (see Figure 4c), indicating the description of the block surface with larger size needs more 13 harmonics series than the smaller one. This is because The  $E_{Sp}$  of blocks are less than 5 % when n is 14 15 higher than 9, while the  $E_R$  becomes lower than 10 % only for *n* higher than 25. As such, in order to

1 describe accurately the morphological features of the SH reconstructed blocks, the value of n was fixed to

2 25 in the generation of SH series.

3 3.1.3 Generation of random SH series

Random SH series can be determined if a set of random SH coefficients  $a'_n^m$  are generated on the basis of the SH coefficients  $a_n^m$  obtained from the CT scanned blocks. Before the generation of  $a'_n^m$ , the CT reconstructed blocks were normalised to remove the influence of their initial orientations and volumes on the SH coefficients by (a) rotating them to have their principal axes parallel to the global coordinate axes; (b) scaling their volume to a unity.

9 N CT reconstructed blocks were selected as samples for establishing the random SH coefficients. N
10 random numbers r<sub>i</sub>, with sum equal to 1, were initially generated, producing the new normalised random
11 SH coefficients a<sup>'m</sup><sub>n</sub>:

$$a_n^{\prime m} = r_1 \left(\overline{a_n^m}\right)_1 + r_2 \left(\overline{a_n^m}\right)_2 + \dots + r_i \left(\overline{a_n^m}\right)_i + \dots + r_N \left(\overline{a_n^m}\right)_N$$
(16)

where  $(\overline{a_n^m})_i$  is the normalisation SH coefficients of the *i*th selected CT reconstructed block and  $\sum_{i=1}^{N} r_i = 1$ .

Following this procedure, thousands of normalised random blocks with unit volume can be establishedonly by creating sets of random number.

17 3.1.4 Selection of available random blocks

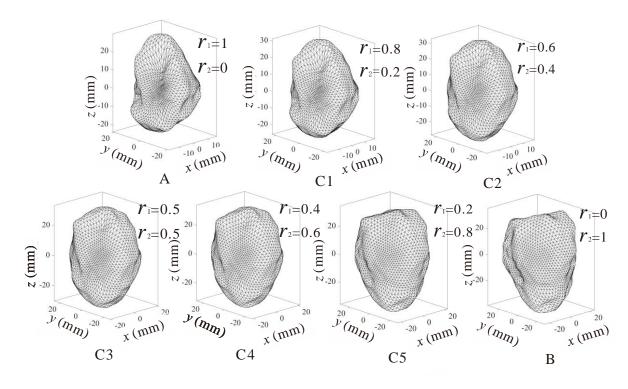
12

The particle size of the normalised random blocks should be modified consistently with that of the real blocks. Accordingly, the same random number set  $r_i$  used in the generation of random SH coefficients was adopted to define the new particle size D' as follow:

21 
$$D' = r_1 D_1 + r_2 D_2 + \dots + r_i D_i + \dots + r_N D_N$$
(17)

22 where  $D_i$  is the particle size of *i*th selected CT scanned block.

Although the random blocks were generated on the basis of the real blocks, some of them are characterised by morphological features not within the ranges identified by the real sampled blocks. For example, Fig. 11 compares the sampled blocks A and B with different random blocks, labelled as C1, C2, C3, C4 and C5.



9

Fig. 11 Random generated blocks based on sample blocks A and B

Random blocks are more similar to block A when  $r_1$  is larger or to block B when  $r_2$  is. The morphological features of the generated blocks are summarised in Table. 1: it is evident that the  $S_P$  and R of C3 and C4 blocks are beyond the range of values identified by the sampled blocks A and B. As such, only the random blocks C1, C2 and C5 can be considered as available while C3 and C4 need to be disregarded.

7 The random blocks were considered as available for the next S-RM model generation only if their
8 morphological features obeyed to all the rules given by Eq. (1), Eq. (3) and Eq. (6).

		-	0		6	•			
Block id	$r_1$	$r_2$	<i>D</i> (mm)	$V (\text{mm}^3)$	<i>S</i> (mm <sup>2</sup> )	EI	FI	$S_p$	R
А	1.0	0.0	42.1	5395.4	27902.3	0.79	0.79	0.82	0.47
C1	0.8	0.2	45.9	6499.3	39475.6	0.80	0.80	0.86	0.50
C2	0.6	0.4	49.6	7750.9	54251.6	0.81	0.79	0.89	0.53
C3	0.5	0.5	53.4	9229.7	72792.8	0.81	0.81	0.91	0.54
C4	0.4	0.6	51.5	8478.5	63272.2	0.81	0.80	0.91	0.54
C5	0.2	0.8	57.2	10590.1	89733.1	0.81	0.81	0.92	0.53
В	0.0	1.0	61.0	11927.3	104028.5	0.82	0.81	0.90	0.53

Table. 1 Morphological features of random blocks generated by block A and B

10

#### 3.2 Stochastic fracture generation approach 1

An example of CT fractures reconstructed in the block was given in Fig. 3b. Considering their complex 2 3D morphological features, difficult to be described precisely, simplified cubic stochastic fracture models 3 were developed on the basis of their statistical characteristics.

3.2.1 Determination of fracture numbers 5

According to the statistical characteristics of real fractures, random fractures were generated only in the 6 7 blocks having a particle size in the range 40 - 80 mm. The number of fractures  $N_{fi}$  in *i*th block can be simply determined by the block volume  $V_i$  considering the average fracture frequency of real fractures (i.e. 8  $10^{-4}$  per 1 mm<sup>3</sup>). As such, the total number of random fractures  $N_{ft}$  is: 9

10 
$$N_{fi} = \sum_{i=1}^{M} N_{fi} = \sum_{i=1}^{M} INT(V_i \times 10^{-4})$$
 (18)

where INT is a function that approximate the resulting value to the nearest integer. M is the number of 11 blocks with size between 40 mm and 80 mm in the S-RM sample. 12

13 3.2.2 Determination of characteristics of random fractures

The relative orientations of random fractures were created on the basis of real ones. A set of random 14 numbers  $\theta_j$  ( $1 \le j \le N_{ft}$ ) were generated to obey an Amplitude Gaussion distribution having the same mean 15 16  $\mu$  and standard deviation  $\sigma$  of the  $\theta$  distribution of scanned fractures. The offset  $y_0$  and amplitude A were scaled on the basis of the number of scanned fractures N and generated random ones M in the S-RM 17 18 sample. As such, the  $\theta_i$  distribution reads:

$$F_{f} = \frac{M \times \left(26.8 - 1441.5 \bullet \frac{1}{\sqrt{2\pi} \bullet 22.7} e^{\frac{(\theta - 70.2)^{2}}{2 \bullet 22.7^{2}}}\right)}{N} , \quad 0^{\circ} \le \theta \le 180^{\circ}$$
(19)

4

Similar to the process of generation of the random fracture orientations, the  $l_{fa}$  values of random fractures, 20 21 ranging from 2 mm to 16 mm, were also created on the basis of the corresponding  $l_{fa}$  distribution of the 22 scanned fractures, expressed in Eq. (7). Based on the  $l_{fa}$  distribution, a random  $l_{fa}$  set  $A_j$  was generated for representing the  $l_{fa}$  dimension of *j*th random fracture. 23

24 3.2.3 Determination of available  $l_{fb}$  and  $l_{fc}$ 

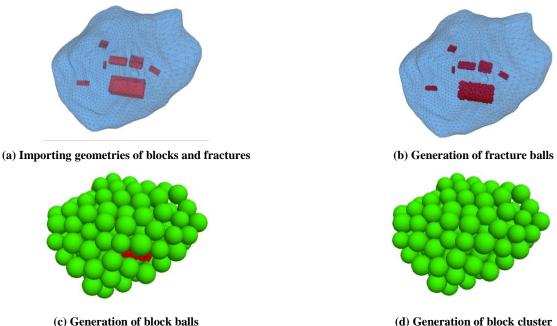
Based on the  $l_{fb}$  dimension of scanned fractures, another set of number  $B_j$  was also randomly generated in 25 26 the interval 1.5 - 12 for representing the  $l_{fb}$  dimension of *j*th random fracture. If the relationship between

27  $B_j$  and  $A_j$  was found to fit in the range indicated by the Eq. (8) valid for the corresponding  $l_{fb}$  and  $l_{fa}$  dimensions,  $B_j$  was considered as an available random number; otherwise, a new random number was created until it conformed to this law. A similar procedure was adopted for the random generation of a series of  $C_j$  values in the interval from 0.7 to 8, representing the  $l_{fc}$  dimension of *j*th random fracture, ensuring that each value satisfied the limits imposed by Eq. (9) with respect to  $A_j$ .

5 3.3 Generation approach for block DEM models

The commercial software Particle Flow Code in three-dimensions (PFC<sup>3D</sup>5.0) was employed to create blocks and S-RM DEM models. The cluster, used to simulate the block, consists of a group of bonded balls with a specified bond strength, commonly used to simulate breakable geomaterials with a certain strength. A cluster behaves as a deformable body, contact forces being generated and updated during the analysis; it breaks once its bond strength is reached. The block DEM model was generated following the next steps:

- (a) *Importing block and fractures geometries*. A block geometry generated by the stochastic block generation approach was imported and the necessary number of random fractures was determined.
  The fracture geometries were selected from the total *M* generated stochastic fractures and imported in the block. The spatial distribution of the fractures were assumed to be randomly distributed within the block; however, a regeneration step was performed if the fractures were found to intersect the surface of block (Fig. 12a).
- (b) *Generation of fracture balls*. Considering that the minimum size of the fractures are only 0.8 mm, the
   minmum radius of fracture balls were set as 8 times less than that of fractures. Balls with radius of 0.1
   0.15 mm were generated in each fracture to fill it completly (Fig. 12b).
- (c) *Generation of block balls*. In order to reflect the block morphological features, the maximum radius
  of block balls were set as 10 times less than that of blocks. Block balls with a porosity of 0.35 were
  generated in the block without the position occupied by the fractures. After fixing all fracture balls,
  the boundaries of all the geometries were taken as the wall boundaries and the analysis was started
  until a balanced state was reached in the assembly (Fig. 12c).
- (d) *Generation of block cluster.* After generating block balls, the fracture balls were all deleted and the
  block balls were fixed at their position. Then the block cluster model was finally generated by
  bonding the block balls with each others by a specified strength (Fig. 12d).



(c) Generation of block balls Fig. 12 Generation process of the block DEM model

## 2 4 Generation of 3D random S-RM DEM models

The *VBP* of the investigated S-RM samples, introduced in Section 2.1, was in the range of 35% - 60%. In particular, the numerical approach will be developed with reference to a S-RM sample characterised by a *VBP* of 40%, for which the results of a large direct shear test are available for the sake of comparison.

6 4.1 Generation of block assembly

Based on the grain size distribution of rock blocks identified experimentally, a total number of 4085
random blocks was generated following the proposed stochastic block generation approach (Table 2).
Similarly, 2335 random fractures were also created for blocks with size of 40 - 80 mm.

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1

Table. 2 Generated rock blocks according to different stes of size dimension

Block Size	10 - 20 mm	20 - 40 mm	40 - 60 mm	60 - 80 mm
<i>VBP</i> (%)	3.1	12.5	14.4	10
Volume (mm <sup>3</sup> )	3077200	12308800	14155120	9847040
Number	3100	702	198	85

The block DEM assembly was generated following two steps (Fig. 13a): (a) first, the shear box employed in the laboratory tests, consisting of a cylinder with a diameter of 560 mm and a height of 400 mm, was introduced; (b) then, the generated block DEM models were imported in the shear box one by one with random spatial and orientation distributions. In order to avoid block overlapping, the block models were 1 set as independent clumps, separated later after some calculation steps.

2 4.2 Generation of S-RM models

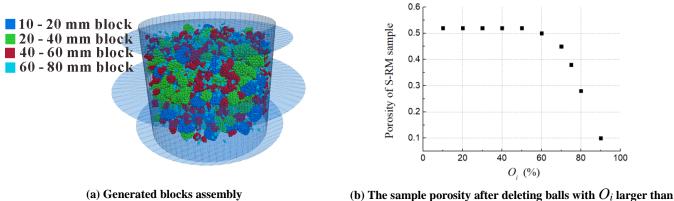
13

In the S-RM sample, particles with size lower than 10 mm are considered as soil particles (i.e. matrix). Considering of the limitation of the computation capacity, the soil particles were simplified as sphere balls having radii from 4.8 mm to 5.0 mm for representing the soil particles in the DEM model. Although the morphology of soil particles can be represented by bonding several smaller balls, this will lead to a large increase in the particle number in the DEM model. As such, the irregular morphology of soil particles was neglected and the rolling resistant model was adopted for simulating their roughness (Jiang et al. 2005, Xu et al. 2016b).

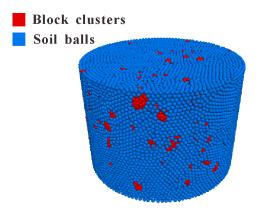
However, the generated soil balls were characterised by a large overlap within the block clumps. The maximum degree of overlap  $O_i$  of *i*th soil ball with the surrounding balls in the block clumps can be expressed as follow:

$$O_{i} = max \ 1 - \frac{D_{sb}}{r_{si} + r_{bj}}) \times 100\% \ (j = 1, 2, ..., N_{cb})$$
(20)

where  $D_{sb}$  is the distance from the centre of *i*th soil ball to that of *j*th block ball.  $r_{si}$  and  $r_{bj}$  are the radii of 14 15 *i*th soil ball and *j*th block ball, respectively.  $N_{cb}$  is the total number of clump balls in the S-RM model. Soil balls with a  $O_i$  larger than a selected threshold (e.g. 10 %, 20 %, 30 %, 40 %, 50 %, 60 %, 70 %, 16 75 %, 80 % and 90 %) were then deleted from the model and the porosity of the S-RM sample was 17 recalculted after balancing the model. As shown in Fig. 13b, after deleting the soil balls with  $O_i$  larger 18 than 75%, the porosity of the S-RM sample reached the required value, equal to 0.38. The final resulting 19 20 3D S-RM DEM model with 40% VBP was then established by transferring the block clumps into clusters 21 and bonding the balls in the clumps with a specified strength value (Fig. 13c).

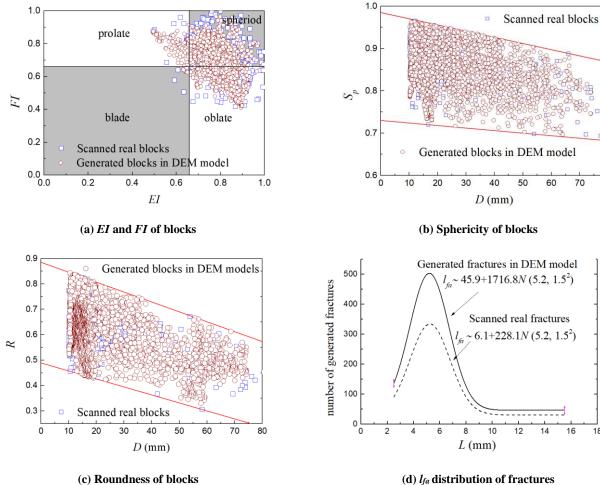


specified values



(c) Generated S-RM DEM model Fig. 13 Generation process of S-RM DEM model

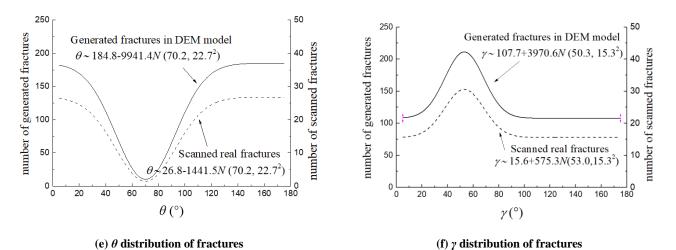
The block morphological features and fracture characteristic distributions of the generated S-RM DEM model are provided in Fig. 14, demonstrating that thousands of random blocks and fractures can be reasonably produced for generating S-RM models on the basis of a limited number of scanned blocks and fractures using the proposed stochastic generation approaches. 

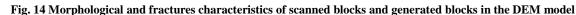


(d) *l<sub>fa</sub>* distribution of fractures

ں لـ 18

 number of scanned fractures





## 1

2 4.3 Determination of meso-parameters

Macro-mechanical properties (e.g. elasticity modulus, cohesion and friction angle) of DEM models are commonly represented by the meso-parameters of particles (e.g. stiffness, friction coefficient and bond strength). Rolling resistant model was adopted for simulating the soil mechanical behaviours, while the parallel bond model was used to represent the mechanical behaviour of breakable blocks.

7 4.3.1 Meso-parameters of soil particles

To obtain the meso-mechanical parameters of the S-RM matrix, particles with diameter less than 10 mm were sieved from the S-RMs to perform large laboratory DSTs. During the tests, the applied normal stresses were 100 kPa, 200 kPa, 300 kPa, 400 kPa and 500 kPa.

About 78,000 soil particles with radius of 4.8 mm - 5 mm were generated in a DEM model having the same size of the large soil DST, and numerical tests were performed under the same normal stresses. The parameters of soil particles used in the DEM simulations are summarised in Table 3.

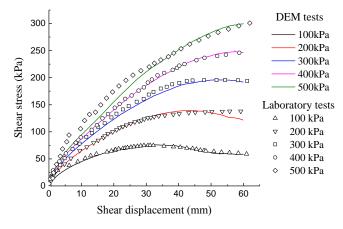
Inspection of Fig. 15a reveals a very good match between experimental and numerical shear stress - shear displacement curves. Interpretation of numerical results provided a cohesion and friction angle respectively equal to 21.4 kPa and 29.6 °, very close to the values obtained from laboratory tests, namely 20.8 kPa and 29.6°. As such, it was demonstrated that the meso-parameters selected for the soil particles are appropriate for representing the soil mechanical behaviours in DEM simulations.

19 4.3.2 Meso-parameters of block clusters

To obtain the meso-parameters of block clusters right on the basis of the block geometries, one CT scanned block with a particle size of 64 mm was selected for performing an uniaxial compression test using a servo test system (Fig. 15b). In particular, an axial displacement rate of 0.002mm/s was adopted. The same test was simulated numerically on a block cluster, generated considering the geometry of the tested block and having internal fractures with the meso-parameters given in Table 3 (Fig. 15c). Fig. 15d shows the good agreement between the numerical and experimental simulations, indicating that the selected meso-parameters allow to well reproduce the mechanical behaviour of blocks.

5 In the S-RM model, the contacts between the soil and block particles obey to a rolling resistance model.

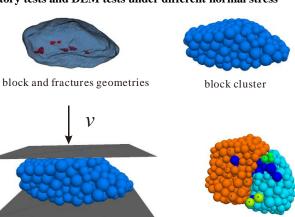
6 The meso-parameters of the contacts between soils and blocks are summarised in Table 3.



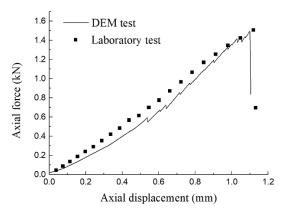
(a) Shear stress vs. shear displacement curves of soil laboratory tests and DEM tests under different normal stress



(b) Laboratory unaxial compression test of single block



numerical compression test of single block failure pattern of block (c) DEM unaxial compression test of single block



(d) Axial force vs. axial displacement of laboratory and DEM compression test of single block Fig. 15 Laboratory and DEM tests of soil and single block

Material	Parameter	Value
	Density of particles (kg/m <sup>3</sup> )	1850
	Damp of particles	0.2
	Elastic modulus of particle contacts (MPa)	10.0
Soil particles	Poisson's ratio of particle contacts	0.5
	Friction coefficient	0.5
	Rolling resistance coefficient	0.05
Block particles	Density of particles (kg/m <sup>3</sup> )	2500
	Damp of particles	0.2
	Elastic modulus of particle contacts (MPa)	110.0
	Poisson's ratio of particle contacts	0.5
	Friction coefficient	0.65
	Bond tensile strength (MPa)	1.5
	Bond shear strength (MPa)	1.5
Contacts between	Elastic modulus of contacts (MPa)	110.0
	Poisson's ratio of contacts	0.5
soil and blocks particles	Friction coefficient	0.65
purcheres	Rolling resistance coefficient	0.10

Table 3 Meso-parameters of materials used in S-RM models

## 2

## **3 5 S-RM numerical tests**

- 4 5.1 Numerical direct shear tests
- 5 5.1.1 Simulation process

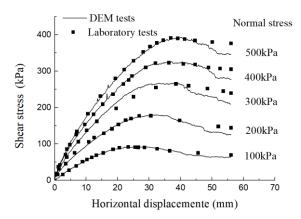
Direct shear tests performed in laboratory ((i.e. with normal stresses of 100 kPa, 200 kPa, 300 kPa, 400 6 kPa and 500 kPa) were simulated consistently with the generated DEM sample. This latter was initially 7 consolidated under the specified normal stress, by controlling the velocity of the top wall of the shear box 8 until the applied normal stress reached the target value. Then, shear loading was applied by moving 9 horizontally the upper shear box wall, with a displacement rate of 0.1 mm/s, slow enough to ensure the 10 sample remains in quasi-static equilibrium (i.e. Cho et al, 2008), while fixing the lower one. When the 11 horizontal displacement reached 56 mm (i.e. 10% of shear strain), the shear test was considered as 12 concluded. 13

1 During the shearing, the shear stress, normal stress and horizontal and vertical displacements were 2 monitored and recorded automatically, as well as the number of meso-cracks, corresponding to the 3 rupture of the bond between the block particles.

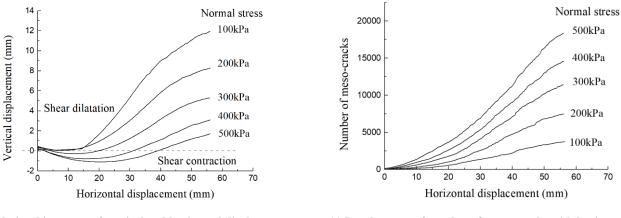
4 5.1.2 Numerical tests results

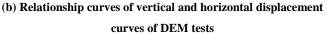
5 The shear stress - horizontal displacement curves of DEM and laboratory tests are compared in Fig. 16a. 6 Before the peak strength, experiments and simulations were found to be in close agreement. However, the 7 reduction in shear strenght was more pronounced in the DEM tests, possibly because a large number of 8 blocks only broke after the peak value and the resulting fragments, being spherical, have a lower 9 angularity than that of the real material.

As shown in Fig. 19b, when the applied normal stress was lower than 200 kPa, dilation occurred during the shearing stage, while the pattern changed from contraction to dilation for normal stresses higher than 300 kPa. The number of meso-cracks generated in the blocks increased rapidly with the horizontal displacement, the process being more pronounced for higher applied normal stresses (Fig. 19c).



(a) Shear stress-horizontal displacement curves of DEM tests and laboratory tests





(c) Development of number of meso-cracks with horizontal displacement of DEM tests

Fig. 16 Tests results of DEM tests and laboratory tests under different normal stress

1 5.2 Evolution of S-RM deformation and failure processes

As shown in Fig. 17, the evolution of S-RM deformation and failure processes can be divided into three stages: the compaction stage, the yield stage and the failure stage. The three stages are described as follows.

5 (a) Compaction stage (stage O-A)

6 With the increase in horizontal displacement, the vertical contraction increased and attained the peak 7 value when the horizontal displacement reached point A (Fig. 17a). The rate of shear stress increment had 8 a small reduction, owing to a small amount of meso-cracks, mainly caused by tensile forces, generated in 9 the S-RM sample (Fig. 17b). The few generated meso-cracks were found to be scatteredly distributed in 10 the S-RM sample, and no broken blocks were still observed at this stage (Fig. 18a).

When horizontal displacement reached point A, only some soil paricles close to the lateral shear box rotated (Fig. 18a), indicating that the shear surface began to develop along the rotated soil particles from the upper right and lower left corner of shear box.

14 (b) Yield stage (stage A-B)

During this stage, the rate of shear stress increment experienced a significative reduction, and a large number of meso-cracks, especially tensile ones, generated in the blocks. Peak strength was attained at point B: as shown in Fig. 18b, some blocks in the centre of the sample displayed an obvious rotation, producing a change in the vertical displacement from contraction to dilation.

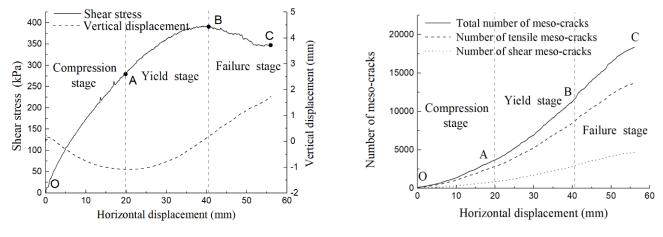
A localization band was observed from the rotation distribution of the particles (Fig. 18b). In addition, some rotated blocks were broken at this stage, indicating that shear surfaces started developing, from the lateral sides of the shear box to it centre, and connecting, by rounding the blocks or even penetrating through them.. The localization band formed with vertical thickness of 9.8 mm.

23 (c) Failure stage (stage B-C)

The failure stage was characterised by a decrease in the shear stress after the peak related to the large number of meso-cracks and the breakage of blocks. Many blocks in the centre of sample were subjected to a large rotation, producing a further dilation of the S-RM sample.

The rotated blocks and soil particles distributed in the centre of sample with a larger vertical thickness of 13.2 mm when the displacement reached point C, characterised by a well developed localization band

29 (Fig. 18c).



(a) Evolution of shear stress and vertical displacement

1

(b) Evolution of meso-cracks number

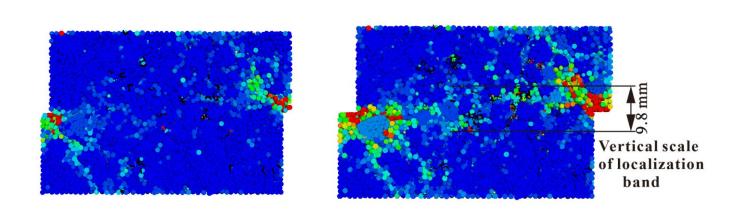
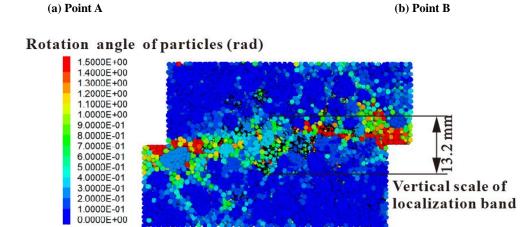


Fig. 17 Evolution of shear stress, vertical displacement and meso-cracks number of S-RM sample under 500kPa normal stress





2 Fig. 18 Evolution of particle rotation and meso-cracks in the middle section of S-RM model under 500kPa normal stress 3 ( the rotation angle is clockwise angle of particles; the black short solid lines are the generated meso-cracks in the blocks)

5.3 Shear strength of S-RM 4

In order to analyse the influence of the block breakage and the presence of internal fractures on the shear 5 6 strength of S-RMs, two new sets of S-RM models were created : (i) S-RM models with unbreakable

blocks, generated by replacing the block clusters with block clumps (see Table 4), with the same soil
meso-parameters of original ones; (ii) S-RM models with breakable blocks but without internal fractures,
adopting the same meso-parameters of soil and block clusters of the original S-RM models.

4

Table 4 Meso-parameters of block clumps used in S-RM models with unbreakable blocks

Parameter	Value
Density of clumps (kg/m <sup>3</sup> )	2500
Damp of particles	0.2
Elastic modulus of clump contacts (MPa)	110.0
Poisson's ratio of clump contacts	0.5
Friction coefficient	0.65
Rolling resistance coefficient	0.10

#### 5

6 The shear strength resulting from the two new sets of simulations is compared to the original one in Fig. 7 19. As expected, the shear strength of the unbreakable S-RM samples was the highest one, indicating the 8 role played by breakable blocks, especially at high normal stresses. Consideration of internal fractures in 9 the breakable S-RM significantly reduced the shear strength of breakable S-RM, demonstrating the 10 importance of this feature in the S-RM modelling.

It was also found that neglecting the possible block breakage and the presence of internal fractures strongly affects the calculated strength parameters of the S-RM. The cohesion c of unbreakable S-RM samples was lower than that of the breakable ones while its friction angle  $\varphi$  was higher. A similar trend was observed in those models not accounting for the presence of internal fractures.

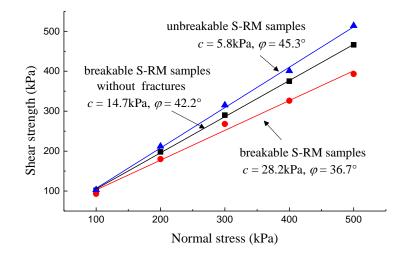




Fig. 19 Shear strength of breakable and unbreakable S-RM samples

## 1 Conclusions

2 This study proposes stochastic approaches for generating block and fracture models, accounting for
3 morphological features and internal fracture characteristics of breakable blocks, to be adopted in the
4 setting up of 3D S-RM DEM models.

The research takes its cue from the case-history of an artificial S-RM filling slope, mainly containing 5 highly-weathered shale blocks, located in the Funing County, Yunnan Province, China. The 3D 6 morphological features of shale blocks and the characteristics of their internal fractures were obtained by 7 CT technology and image processing. Stochastic block generation methods were developed on the basis 8 of SH series of real blocks for establishing random blocks DEM cluster models. Similarly, random 9 fracture models, simulated as voids in the block clusters, were created by a stochastic generation approach 10 11 on the basis of real fracture characteristic distributions. The attention was focused on a 3D modelling of a S-RM with 40% VBP, by setting reasonable meso-parameters. Its mechanical behaviour during numerical 12 13 direct shear tests was analysed in detail, to investigate the mechanisms of shear band development and localisation and the role played by block breakage and internal fractures. 14

15 The following main conclusions can be drawn:

(1) The shale blocks were mainly spheroidal and their sphericity was found to be in the range of 0.7 - 0.97,
typically larger for the smaller blocks. The roundness of blocks varied from 0.3 - 0.8, the larger blocks
having a higher angularity than the smaller ones. The average frequency of real fractures was 0.1 per
1 cm<sup>3</sup> in the blocks with size of 40 - 80 mm. The size and orientation distributions of fractures were
both found to obey the Amplitude Gaussian laws.

(2) In the random block generation approach, the SH degree of blocks *n* was accurately determined on the
basis of the block morphological features, fixed to 25 for the generation of random SH series. The
distributions of random fracture sizes and orientations were also reasonably determined on the basis
of those of real fractures. Thousand random blocks and fractures with similar morphological features
and characteristic distributions to real ones were produced in the S-RM DEM models using the
developed stochastic block generation approach.

(3) The comparison between the results of DEM and laboratory direct shear tests demonstrated that the
 generated random S-RM DEM models and the selected meo-parameters can be reasonably used for
 reproducing the mechanical behaviour of S-RM samples with breakage blocks.

(4) The evolution of S-RM shearing process can be subdivided into three stages: the compaction stage,
the yield stage and the failure stage. The shear surface formed from the lateral shear box to the centre
of sample during the compaction stage; then it connected by rounding the blocks or even penetrating
through them, producing a localization band with rotated blocks in the yield stage; finally, the
localization band developed with a larger vertical scale at the failure stage. The breakage of blocks
mainly occured in the localization band, mostly casued by tensile forces.

7 (5) It was also demonstrated that neglecting block breakage and the presence of internal fractures had
8 significant influence on the shear strength of the S-RM model, by increasing its shear strength and
9 friction angle while reducing its cohesion.

10 The stochastic generation approach can be also used for establishing other S-RM samples with different 11 block morphological features, block volume proportions and fracture distributions. The influence of all 12 these factors on the S-RM mechanical behaviour is the object of future research.

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- 26 27

# **Author Statement**

The all authors' individual contributions are as follows:

Xinli Hu: Project administration, Funding acquisition, Supervision;

Han Zhang: Conceptualization, Methodology, Software; formal analysis, Data Curation, Investigation, Resources and Writing- Original draft preparation;

Daniela Boldini: Writing - Review & Editing, Validation, Supervision;

Chang Liu: Data Curation and Software;

Chuncan He: Investigation and Resources;

Shuangshuang Wu: Writing - review & editing.

## **Declaration of interests**

 $\boxtimes$  The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

□ The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: