

1 **Spatial vector characterization of intra-particle pore structures for**
2 **carbonate sand particles**

3 Yi-Hang Wu,¹ Bei-Bing Dai, Ph.D.,² Yi-Pik Cheng, Ph.D.,³ Jun Yang, Ph.D., F.ASCE⁴

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5 ¹Ph.D. student, School of Civil Engineering, Sun Yat-sen University, Guangzhou, China,
6 510275; and Department of Civil, Environmental and Geomatic Engineering, University
7 College London, London, United Kingdom, WC1E 6BT; E-mail: wuyh239@mail2.sysu.edu.cn

8 ²Professor, School of Civil Engineering, Sun Yat-sen University, Guangzhou, China, 510275;
9 State Key Laboratory for Tunnel Engineering, Guangzhou, China, 510275; and Southern
10 Marine Science and Engineering Guangdong Laboratory (Zhuhai), Zhuhai, China, 519082; E-
11 mail: daibb@mail.sysu.edu.cn (Corresponding author)

12 ³Associate professor, Department of Civil, Environmental and Geomatic Engineering,
13 University College London, London, United Kingdom, WC1E 6BT; E-mail:
14 yi.cheng@ucl.ac.uk

15 ⁴Professor, Department of Civil Engineering, The University of Hong Kong, Hong Kong, China,
16 999077; E-mail: junyang@hku.hk

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Abstract

19 This paper presents an investigation of the spatial distribution of intra-particle voids in
20 carbonate sand particles using X-ray micro-tomography (μ CT) to obtain high-resolution 3D
21 particle images. A vector representation approach is introduced within a statistical
22 micromechanics framework to characterize the spatial organization of internal pore structures.
23 The study establishes a tensor formulation based on pore orientation vectors and volume-
24 weighted pore orientation vectors to quantify the anisotropic distribution of intra-particle pores.
25 It is found that volume-weighted pore orientation vectors exhibit a considerably higher degree
26 of anisotropy than pure pore orientation vectors. For highly porous particles, the anisotropic
27 distribution of volume-weighted pore orientation vectors is largely governed by the presence
28 of a dominant open pore, aligning the principal pore anisotropy direction with the overall
29 particle orientation. Moreover, a dependence of porosity, pore diameter, and the anisotropy
30 parameter a_v on particle size is observed, while the pore shape parameter (aspect ratio) remains
31 size-independent. The relationships between pore structure characteristics and particle skeleton
32 morphology are explored, revealing that correlations, such as those between sphericity, porosity,
33 and pore anisotropy, are not strictly interdependent, depending on factors like pore connectivity
34 and size. These findings provide new insights into the micromechanical behavior of carbonate
35 sand particles and their influence on hydraulic transport properties.

36 **Keywords:** carbonate sands; internal pores; spatial distribution; anisotropy; X-ray μ CT; vector
37 representation

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48 **1. Introduction**

49 Carbonate sands are a kind of natural sands derived from marine biological remnants (e.g.,
50 corals, mollusk, foraminifera, ooidic and so on) (Coop 1990), which are commonly encountered
51 in offshore engineering construction. The special cavity structure of marine organisms allows
52 carbonate sand particles to retain considerable internal pores and exhibit different mechanical
53 properties from terrestrial silica sand particles (Dong et al. 2024; Giretti et al. 2018; Zhang et
54 al. 2023). The characterization of the internal pore structures, along with their relations with
55 the particle breakage and other mechanical behavior, has garnered increasing attention from
56 researchers (Andò et al. 2013; Fonseca et al. 2012; Karatza et al. 2018).

57

58 For example, Li et al. (2020) observed through in situ micro-CT that the presence of
59 internal pores facilitates the initiation and propagation of cracks, contributing to the reduction
60 of particle failure strength. Lv et al. (2021) used the index of porosity to characterize the overall
61 pore volume within a single particle, and found that particles almost completely lose their
62 strength and stiffness when the porosity exceeds 0.25 in the single-particle compression test.
63 Kuang et al. (2024) employed the porosity and pore fractal dimension to describe the pore
64 characteristic of porous particles in the discrete element method (DEM) simulations, revealing
65 that as these pore descriptors increase, the particle failure mode transits from being brittle to
66 being ductile. Zhou et al. (2020) conducted a comprehensive investigation on the pore size
67 distribution, pore fractal dimension, and the Euler characteristic, and developed the correlation
68 between the pore characteristic indexes and the permeability property. It is obvious that
69 researchers have made significant achievements in characterizing the internal pore structures

70 of carbonate sand particles (e.g., the pore size, pore shape, fractal dimension of pore size
71 distribution, and pore connectivity) and correlating the pore characteristics with the mechanical
72 behavior of sand particles or assemblies (Fan et al. 2021; He et al. 2021; Kong and Fonseca
73 2018; Zhou et al. 2020). However, it seems that in these studies, the scalar parameters are
74 preferred for the characterization of internal pore structures, which cannot capture the spatial
75 distribution characteristics of pore structures.

76

77 Recently, Zhao et al. (2015) has observed through the single-particle compression test that
78 the spatial location of weak points (i.e., the internal pores and impurities) in a particle plays an
79 important role in determining the crack initiation and propagation path, as well as the particle
80 fracture mode. Similarly, Zhou et al. (2022), using the numerical simulation based on a
81 combined finite-discrete element method (FDEM), found that a specific location where an
82 intra-particle pore is present tends to suffer from an intense stress concentration, which is
83 mainly responsible for the initiation and progression of cracks. In addition, Ma et al. (2021)
84 revealed that varying the pore orientations leads to the variation of the permeability levels, even
85 under an identical pore volume. Such studies have clearly demonstrated that the spatial
86 distribution of internal pore structures can exert an unignorable effect on the mechanical
87 behavior (e.g., the particle breakage and permeability) of carbonate sand particles. It is also
88 noted that the current method of characterizing the pore structures within particles based on the
89 scalar representation cannot thoroughly describe the spatial distribution characteristics, which
90 has limited a comprehensive and accurate understanding of the mechanical behavior of
91 carbonate sands.

92

93 In this context, this study focuses on the characterization of three-dimensional spatial
94 distribution of internal pores in carbonate sand particles, with the use of a vector representation
95 approach. By a careful microscopic analysis of μ CT images, the pore structures are
96 characterized by the pore orientation vector and volume-weighted pore orientation vector in a
97 three-dimensional space. On the basis of vector quantities, a statistical analysis is done to
98 achieve a micromechanical description of internal pore structures in a 3D space. Efforts are also
99 made to investigate the relationship between the pore and solid phase characteristics. It is hoped
100 that this study can provide some new insights into the internal pore structure of carbonate sands.

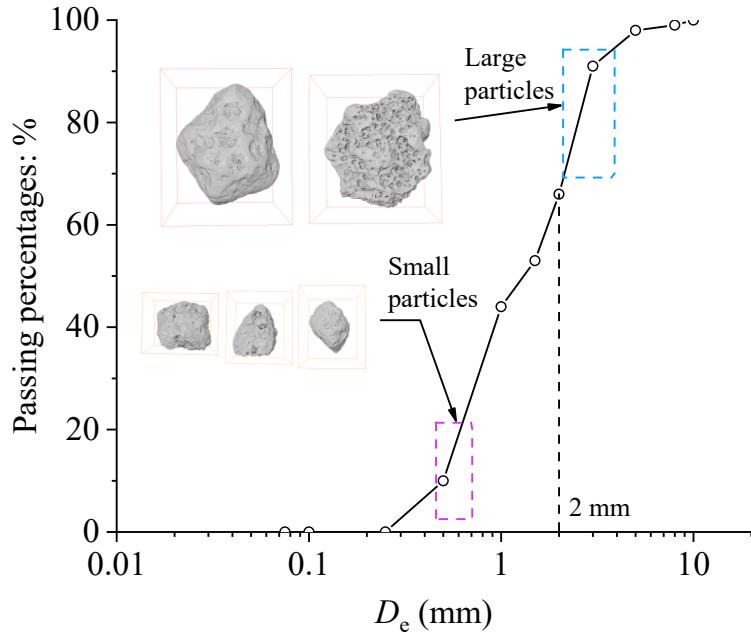
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102 **2. Soil description and digital implementation**

103 *2.1 Test material and methodology*

104 The carbonate sand particles under investigation are a kind of calcareous sediments primarily
105 originating from corals in the South China Sea. The equivalent diameter (D_e) of the sand
106 particles ranges from 0.3 mm to 8.2 mm (see Fig .1), which is given by $D_e = (6V_s/\pi)^{1/3}$, where
107 V_s is the volume of the particle. The particle structures for both the solid and pore phases, were
108 examined using a μ CT system (NanoVoxel 3000) from Sanying Precision Instruments Co., Ltd.

109



110

111 Fig. 1 The particle gradation of carbonate sand particles for testing

112

113 *2.2 Image processing*

114 For the processing of raw image data obtained from scanning, a 3D median filtering algorithm
 115 was employed to reduce the noise generated during scanning. The voxels corresponding to the
 116 solid phase were initially identified using Otsu's thresholding segmentation method (Otsu
 117 1979), which determines the optimal threshold value by maximizing the variance between
 118 distinct phases in grayscale images. This method has been widely recognized for its
 119 effectiveness in distinguishing different phases in CT-reconstructed images (Nishimura et al.
 120 2024; Zhao et al. 2015). Subsequently, the pore phase was determined through the application
 121 of filling algorithms, including the Fill Holes and Ambient Occlusion algorithms. According to
 122 the classification method proposed by Rouquerol et al. (1994), the internal pores within the
 123 particle boundary consist of two components: closed pores and open pores. The Fill Holes
 124 algorithm helps to identify pore voxels surrounded by the solid-phase voxel structure as closed

125 pores (Cheng and Wang 2021; Zhou et al. 2022). The Ambient Occlusion algorithm is used to
126 extract open pores based on the occlusion values of light rays projected from multiple angles
127 (Titschack et al. 2018). Using these image processing methods, the voxel sets for both the solid
128 skeleton and pores were extracted, enabling a further analysis of their size and morphology.
129 The particle and pore volumes are computed by summing the volumes of all corresponding
130 image voxels. While closed pores typically exhibit a spherical or ellipsoidal shape, a big open pore
131 often presents as an inter-connected nest-like unit of pore volume for particles with high porosity,
132 as shown in the subset of Fig. 2, and the size of this cluster is represented by its equivalent diameter
133 mentioned above. Previous studies have shown that the two-dimensional pore shape and
134 orientation can be well captured using the ellipses equivalent to the pore outlines (Gao et al.
135 2020; Zheng et al. 2022). Similar approach was adopted in this study to capture the pore
136 dimensions, with the pores treated as ellipsoids, and some examples for the reconstructed
137 particles and pores are shown in Fig. 2(b). The orientation of the global shape of each pore is
138 determined using the moment of inertia method. The orientation of a pore is represented by a
139 three-dimensional unit vector (see Fig. 2), parallel to the pore's longest axis. This longest axis
140 is treated as its principal axis of inertia, characterized by the eigenvector associated with the
141 largest eigenvalue of the inertia matrix. The dimensions of each particle and pore are
142 determined by the bounding box method, with major (L), intermediate (I) and minor (S)
143 dimensions defined following $L > I > S$ (Huang et al. 2023; Krumbein 1941; Ma et al. 2019).
144 In present study, two morphology parameters, the flatness (FL) and elongation (EL), are
145 calculated, with FL defined as $= I/L$ and EL as S/I . The sphericity (S), describing the degree to
146 which a particle/pore resembles a sphere, is also used to provide a more comprehensive

147 characterization of morphology, and calculated by $S = (36V_s^2)^{1/3}/A$, where A is the surface area
148 of a given particle/pore.

149

150 **3. Quantifying pore fabric**

151 Fabric tensor has been used to describe the spatial distribution of the vector quantities
152 characterizing the microscopic structures and force network in a granular assembly, such as
153 the contact normal/force vector, branch vector, and particle orientation vector (Fonseca et al.
154 2013; Ma et al. 2014; Sitharam et al. 2009; Sun and Zheng 2019; Zhao et al. 2021; Zhou and
155 Xu 2024). Note that unlike the almost continuous void spaces in particle assemblies, the internal
156 pores within a single particle can be regarded as a kind of discontinuities. In a 3D space, the
157 orientation vector of an internal pore, denoted as \vec{n} as indicated in Fig. 2, is described by the
158 horizontal angle (α) and the vertical angle (β). Based on the fabric tensor proposed by Satake
159 (1982) and Ken-Ichi (1984), the 3D spatial distribution anisotropy of the intra-particle pores is
160 expressed as

161
$$\Phi_{ij} = \frac{1}{4\pi} \int_{\Omega} P(\mathbf{n}) n_i n_j d\Omega \quad (1)$$

162 where n_i ($i=1, 2, 3$) is the unit vector of pore orientation, Ω refers to the representative elemental
163 volume (REV), and $P(\mathbf{n})$ is the distribution probability density function. The discrete form of
164 this equation is written as

165
$$\Phi_{ij} = \frac{1}{N_v} \sum_{N_v} n_i n_j \quad (2)$$

166 where N_v is the total number of vectors in a particle, and Φ_{ij} is the fabric tensor for the pore
167 orientations. The probability density function $P(\mathbf{n})$ is expressed as a second-order Fourier
168 series (Guo and Zhao 2013; Ouadfel and Rothenburg 2001; Zhao et al. 2018):

169
$$P(\mathbf{n}) = \frac{1}{4\pi} (1 + a_{ij}^p n_i n_j) \quad (3)$$

170 where a_{ij}^p is a deviatoric and symmetric second-order tensor for the characterization of pore
171 orientation anisotropy. With the substitution of Eq. (3) into Eq. (1), one can obtain

172
$$a_{ij}^p = \frac{15}{2} \Phi'_{ij} \quad (4)$$

173 where Φ'_{ij} is the deviatoric part of Φ_{ij} , with $\Phi'_{ij} = \Phi_{ij} - \delta_{ij} \Phi_{kk} / 3$ (δ_{ij} is the Kronecker
174 delta).

175

176 Note that the distribution of pore volumes in a particle is not uniform; the pores with a
177 larger volume may have a more significant impact on the pore anisotropic distribution. With
178 the consideration of pore volume effect, the volume-weighted pore orientation tensor and the
179 probability distribution function are given as

180
$$\psi_{ij} = \frac{1}{4\pi} \int_{\Omega} V(\mathbf{n}) n_i n_j d\Omega = \frac{1}{N_v} \sum_{Nv} \frac{v_p n_i n_j}{1 + a_{kl}^p n_k n_l} \quad (5)$$

181
$$V(\mathbf{n}) = \bar{v}_0 (1 + a_{ij}^v n_i n_j) \quad (6)$$

182 The deviatoric tensor related to the anisotropic distribution of volume-weighted pore
183 orientation vectors, a_{ij}^v , is defined as

184
$$a_{ij}^v = \frac{15}{2} \frac{\psi'_{ij}}{\bar{v}_0} \quad (7)$$

185 where \bar{v}_0 ($\bar{v}_0 = \psi_{ii}$) is the average pore volume over the entire REV domain with the pore
186 orientation vectors given equal weight at various directions, and this differs from the average
187 volume over all pores.

188

189 The invariants of the deviatoric tensor are conventionally used to quantify the degree of

190 the distribution anisotropy for the pore orientation vector and volume-weighted pore orientation

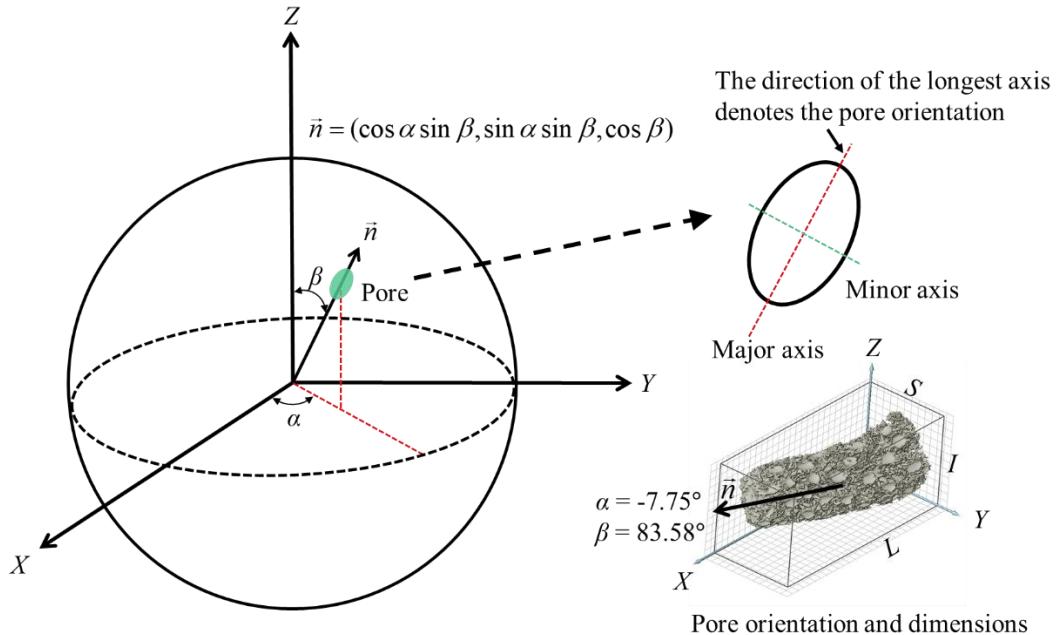
191 vector, which is given by a unified expression:

192

$$a_* = \sqrt{\frac{3}{2} a_{ij}^* a_{ij}^*} \quad (8)$$

193 where the sub/super-script * indicates either the pore orientation anisotropy (p) or the volume-

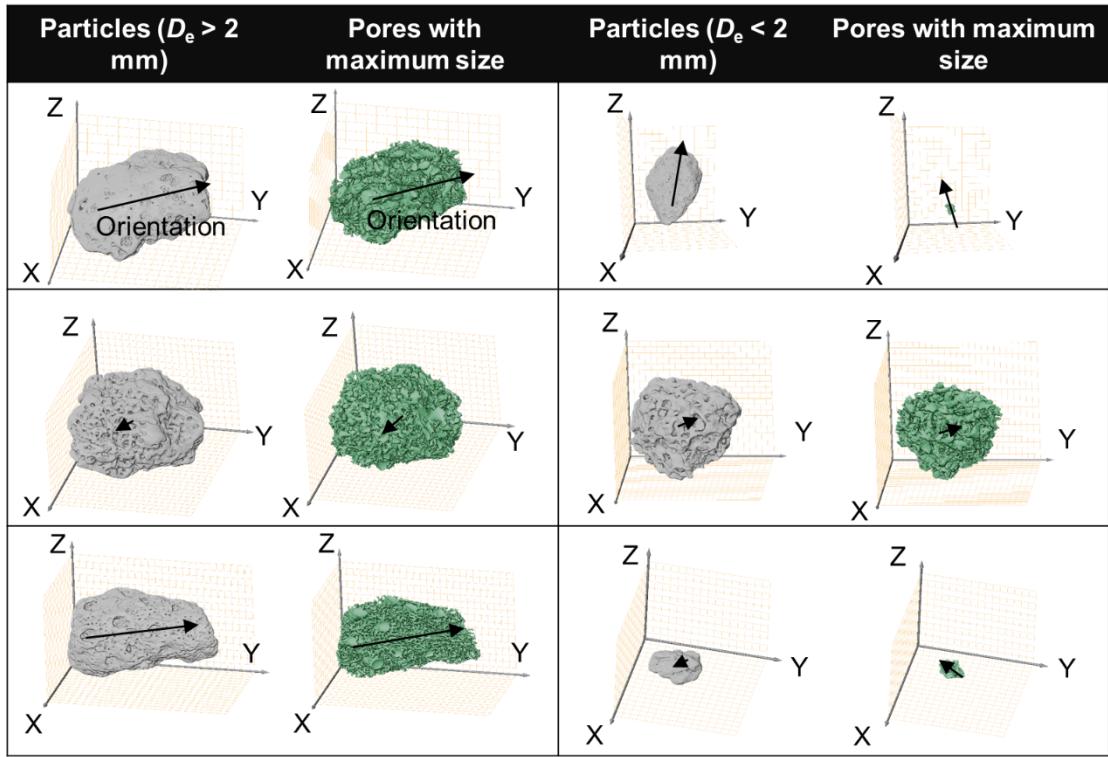
194 weighted pore orientation anisotropy (v).



195

196

(a)



197

198

(b)

199 Fig. 2 (a) Definition of the vector \vec{n} in a unit sphere and (b) examples of reconstructed particles and
200 pores with schematic directional arrows

201

202 **4. Results and analyses**

203 *4.1 Scalar characterization of internal pores*

204 The scalar quantity, porosity (φ), is used here to characterize the volume fraction of the intra-
205 particle pores (including open pores and closed pores) within a particle, which is defined as

206

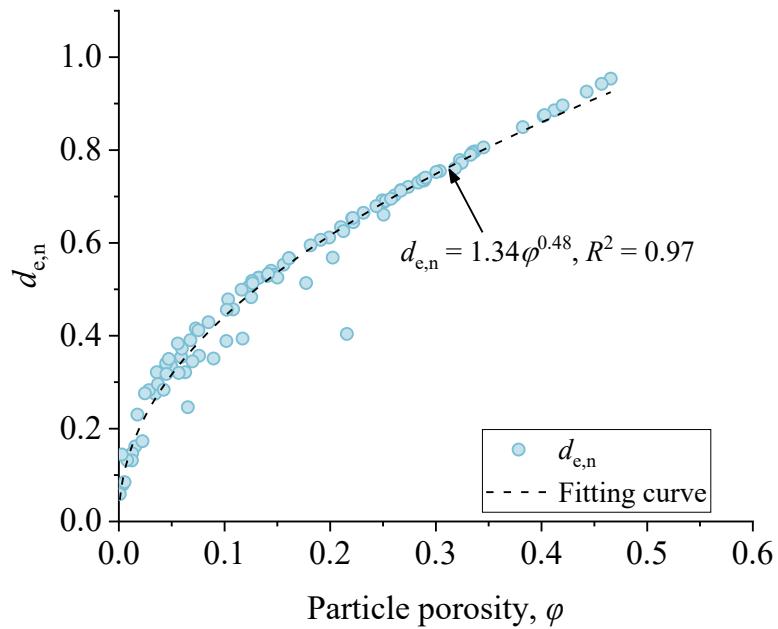
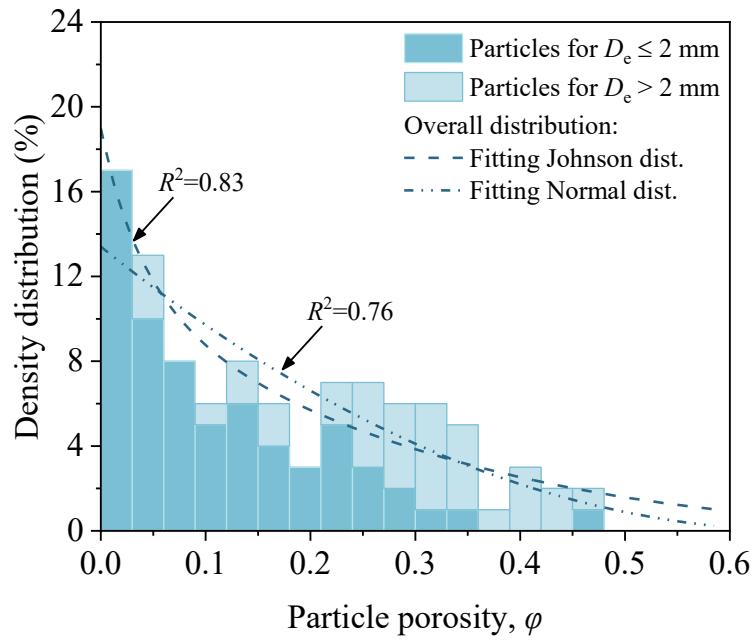
$$\varphi = \frac{V_p}{V_p + V_s} \quad (9)$$

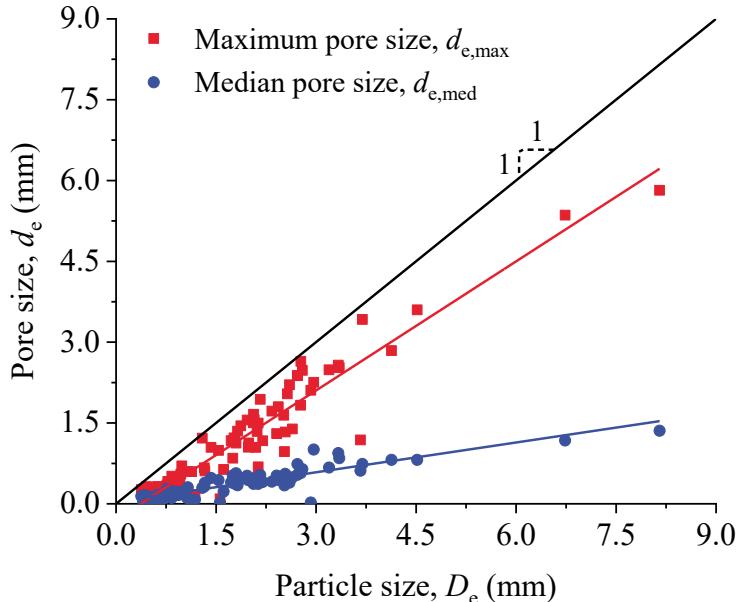
207 where V_p and V_s are the voxel volumes for the pore and solid phases, respectively. Fig. 3
208 illustrates the density distribution of particle porosity along with the fitting curves given by the
209 Johnson distribution and the normal distribution functions. It is observed that the particles with

210 a higher porosity exhibit a lower occurrence probability. Both Gaussian and Johnson
 211 distribution functions were employed to evaluate the distribution curves. The Gaussian
 212 distribution is a commonly used symmetric distribution function, while the Johnson distribution
 213 is well-suited for handling asymmetric cases. The fitting curve of the Johnson distribution
 214 yields similar results but has a slightly higher R^2 value, compared to the normal distribution.
 215 The probability density function (PDF) for the Johnson distribution is given by Johnson (1949)
 216 as

$$217 \quad P(x) = \frac{\delta}{\lambda \sqrt{2\pi}} e^{-\frac{1}{2} \left(\gamma + \delta \sinh^{-1} \left(\frac{x-\xi}{\lambda} \right) \right)^2} \quad (10)$$

218 where ξ , δ , λ , and γ are the function parameters with their values listed in Table 1. Additionally,
 219 the particles with an equivalent diameter (D_e) greater than 2 mm tend to have a higher porosity
 220 than the smaller particles. Fig. 4(a) presents the relationship between the maximum pore size
 221 and the porosity. The normalized maximum pore size ($d_{e,n}$) is defined as the ratio of the
 222 maximum equivalent pore diameter against the equivalent diameter for the solid particle
 223 skeleton. A clear correlation is identified: $d_{e,n}$ increases as a power function with the increasing
 224 porosity, indicating that the particles having a higher porosity are prone to have larger pores
 225 that occupy a significant portion of the total particle volume. Some of the particles have a $d_{e,n}$
 226 up to 0.9. In such cases, the particles would be highly hollow, with pore volumes approaching
 227 the size of the particles themselves. It can be particularly observed in Fig. 4(b), where some
 228 data points for maximum pore size lie close to the diagonal.





(b)

Fig. 4 (a) Relationship between $d_{e,n}$ and φ for the tested carbonate sand particles, and (b) maximum and median pore size against particle size

234

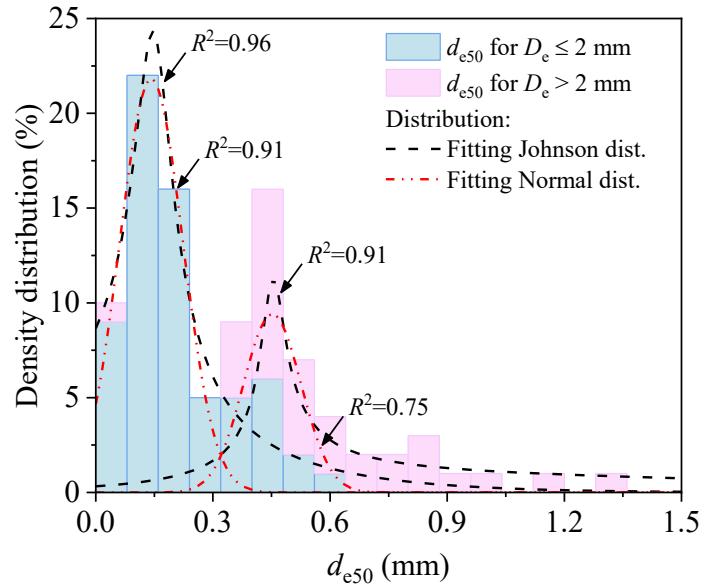
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236 Fig. 4 (a) Relationship between $d_{e,n}$ and φ for the tested carbonate sand particles, and (b) maximum and
237 median pore size against particle size

238

239 Fig. 5 shows the density distribution in terms of pore size and pore shape. The median
240 equivalent diameter, d_{e50} , is used to present a statistical average of the overall pore size in a
241 particle and is calculated by the median value of the cumulative pore size distribution curve. In
242 Fig. 5(a), the Johnson and Gaussian distributions are separately fitted to the data for particles
243 larger and smaller than 2 mm, respectively. It is shown that pore size is positively correlated
244 with particle size, which further supports the observation that larger particles are more prone to
245 breakage (Hardin 1985; Wu et al. 2024). Figure 5(b) reveals that pore shape does not exhibit a
246 clear dependence on particle size, as the aspect ratio of pores exhibits no significant variation
247 across different particle size ranges. For such nearly symmetrical data, the normal distribution
248 function provides a better fit compared to the Johnson distribution.

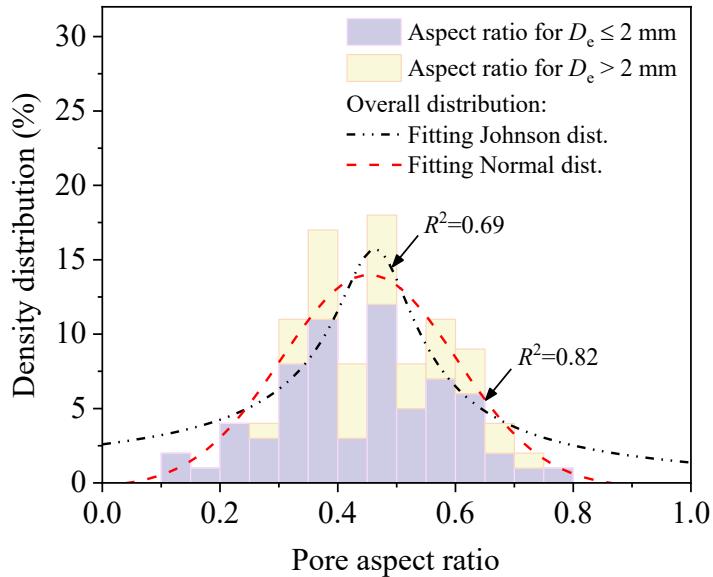
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250

251

(a)



252

253

(b)

254

Fig. 5 Distribution of (a) pore size and (b) pore shape for the carbonate sand particles

255

256 *4.2 Vector characterization of pore orientations*

257 In this section, the pore orientation is brought into focus for a good understanding of the pore
 258 spatial distribution in carbonate sand particles with varying porosities. For an effective

259 characterization of pore orientations in a 3D space, the particle orientations are ensured to align
 260 with the Z-axis in the global Cartesian coordinate system through rotating the coordinate system
 261 by an angle θ_r , as depicted in Fig. 6. Fig. 7 presents the distributions of pore orientations for
 262 four representative carbonate sand particles with the porosity ranging from 1.2% to 22.1%. The
 263 particle with a porosity of 1.2% exhibits a relatively isotropic distribution in terms of both the
 264 pore orientation and volume-weighted pore orientation vectors, as compared with the particles
 265 with high porosities. As the porosity increases, the distribution anisotropy seems to become
 266 more pronounced, particularly for the volume-weighted pore orientation vectors, and this is
 267 primarily due to the presence of a certain number of large pores that could dominate the overall
 268 volume and anisotropic distribution of intra-particle voids. While the pore orientation and
 269 volume-weighted pore orientation vectors in the low-porosity particle basically display similar
 270 angles for the principal anisotropy direction, this has not been observed in the particles with
 271 relatively high porosities.

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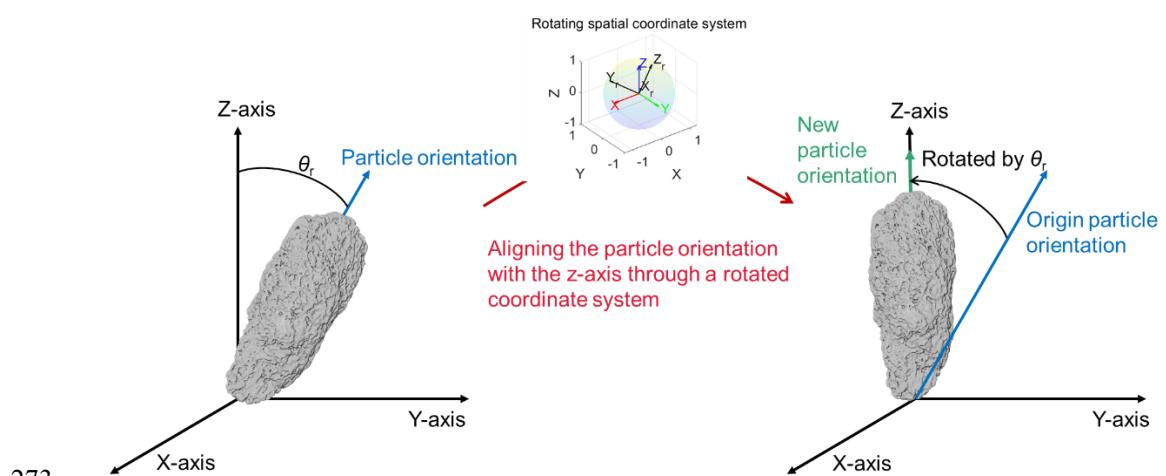
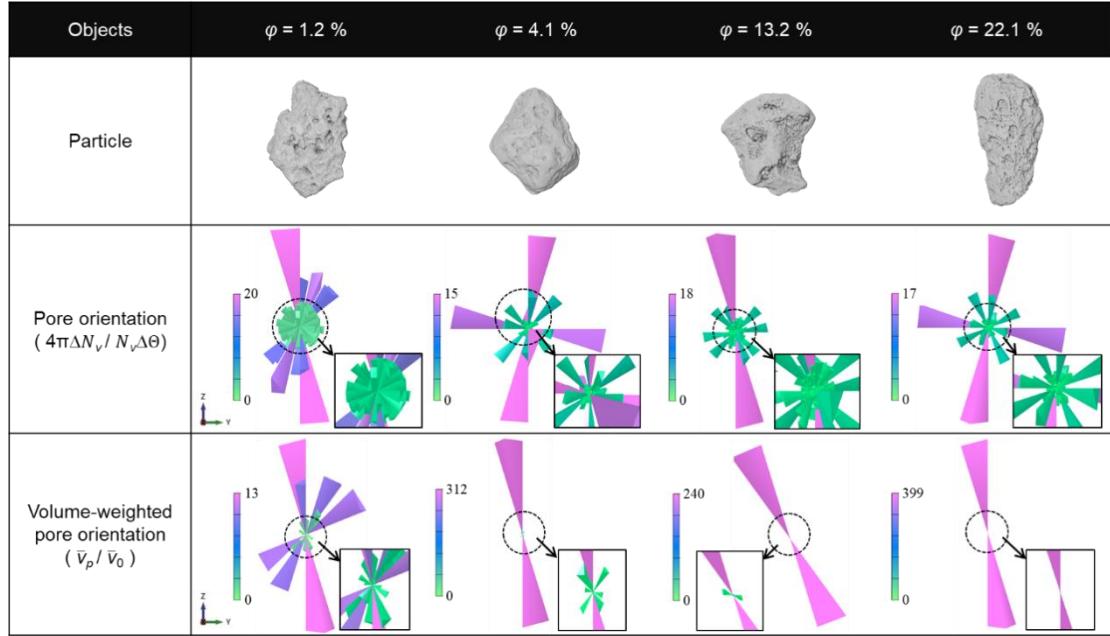


Fig. 6 Schematic diagram of a particle in the rotating coordinate system

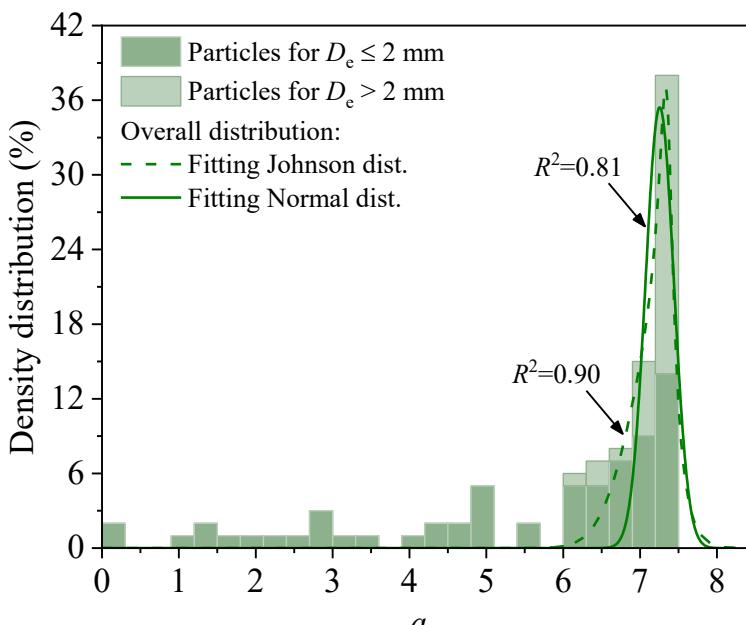
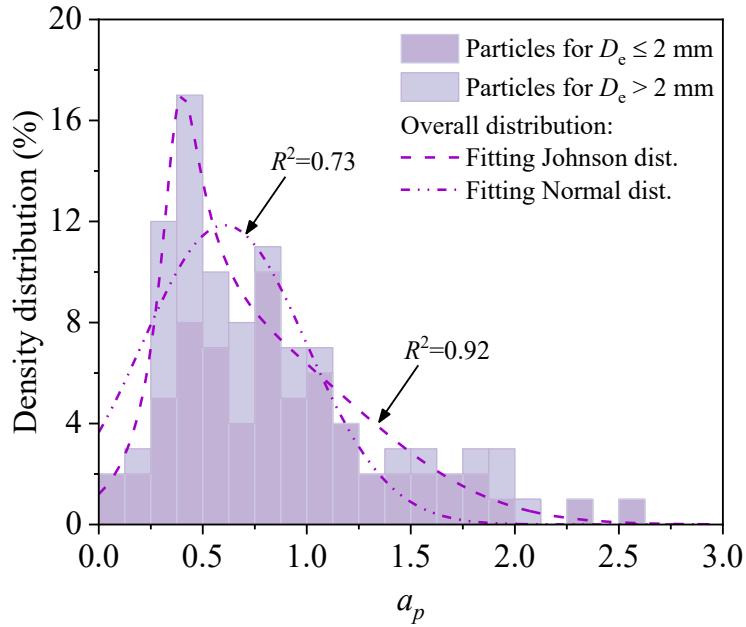


276

277 Fig. 7 3D histograms of the pore orientation of particles with different porosity

278 The pore distribution anisotropy magnitude, given by the invariants a_p and a_v (where a_p
279 denotes the pore orientation anisotropy intensity and a_v represents the volume-weighted pore
280 orientation anisotropy intensity, as defined in Eq. 8), is plotted in Fig. 8. It is seen that the a_v is
281 obviously higher than a_p , indicating that the distribution of volume-weighted pore orientation
282 vectors has a significantly higher anisotropy degree than that for the pure pore orientation vector.
283 Both a_p and a_v demonstrate highly non-normal distribution characteristics. Interestingly, the
284 Johnson distribution can basically more accurately capture the main skewness-kurtosis region,
285 providing a better fit of the pore anisotropy magnitude than the normal distribution.
286 Furthermore, a particle-size dependence of anisotropy magnitude is observed in a_v , and larger
287 particles tend to possess higher a_v values.

288

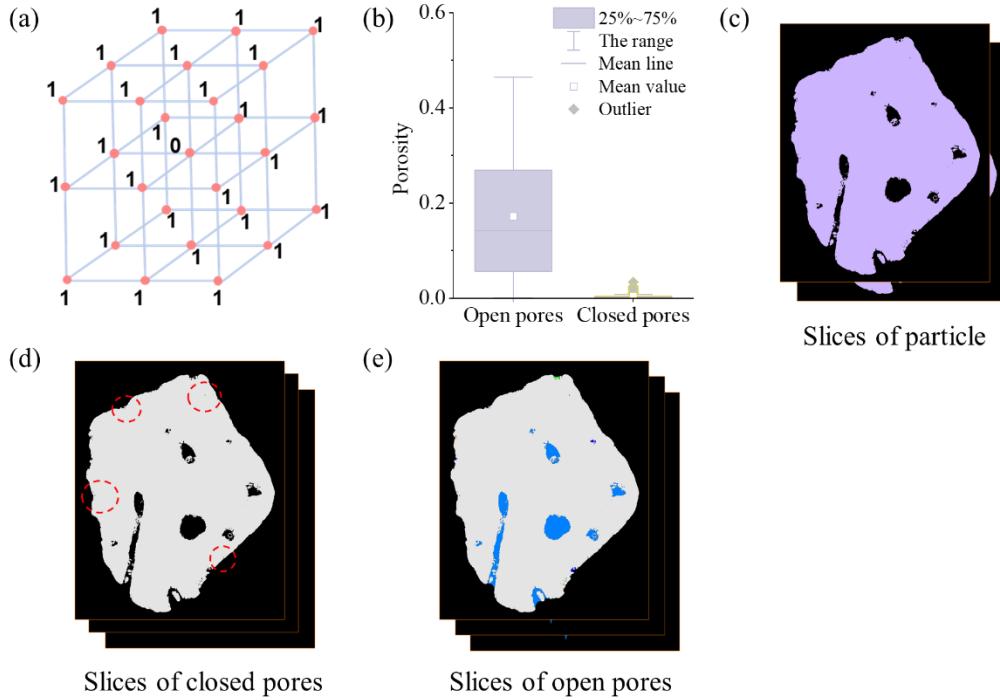


293 Fig. 8 Distributions of (a) a_p and (b) a_v for the tested carbonate sand particles

294

295 To explore more fundamentals of the spatial distribution of pore structures, the internal
 296 pores are classified into open and closed pores. The open pores can directly interact with the

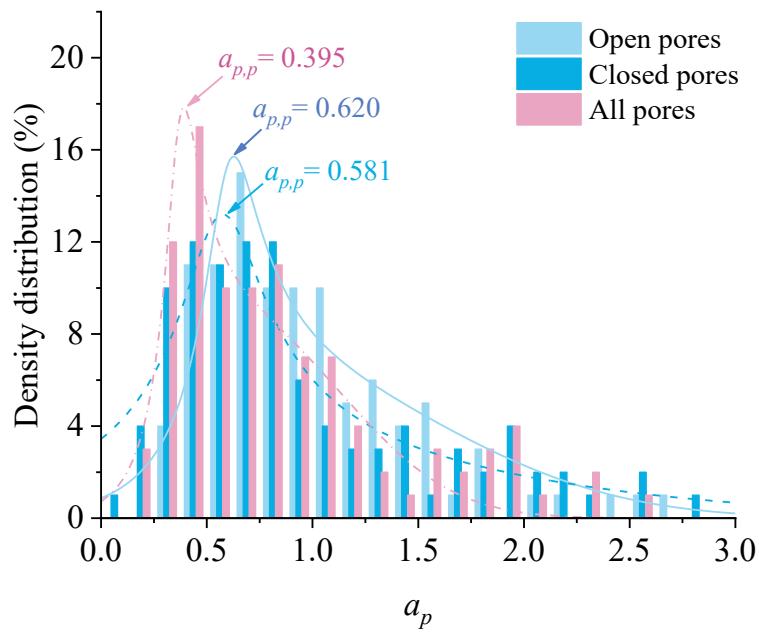
297 external fluids, but the closed pores cannot (Rouquerol et al. 1994; Zhou et al. 2021). In this
298 study, a special algorithm was utilized to differentiate the closed pores from the overall internal
299 pores by picking up the pore voxels surrounded by the solid voxels. As illustrated in Fig. 9(a),
300 this algorithm operates within a three-dimensional space, where a voxel as a void phase (with
301 the point value 0) is identified as a closed pore if all 26 neighboring voxels are labeled as the
302 solid phase (with the point value 1), and 34 neighboring solid voxels in total are needed to be
303 evaluated to identify two voxels of closed pores. Fig. 9(b) provides a comparison of porosity
304 attributed to closed pores and open pores for a typical particle (see Fig. 9(c)), with their
305 corresponding visualizations displayed in Figures 9(d) and 9(e). It can be seen that open pores
306 are substantially larger than closed pores, thus accounting for the majority of the total internal
307 pore volume. Notably, some open pores may appear as closed pores in 2D slices; however, in
308 3D space, these pores are actually connected to the particle's external surface. Fig. 10 shows
309 the variations of the anisotropy magnitudes of a_p and a_v for different pore types, with the general
310 variation trends characterized by the Johnson distribution fitting curves. It is interesting to see
311 that a_v for the open pores is comparable to that for overall pore entities, whereas a_v for the
312 closed pores is distinctly lower. Since a_v has incorporated the influence of pore volume, the
313 similarity in the distribution anisotropy between the open pores and the overall pores suggests
314 that open pores comprise a significant volume fraction of the entire internal pore structure. The
315 peak point of the fitting curve, denoted as $a_{*,p}$, represents the maximum occurrence probability
316 at a particular anisotropy magnitude which is 0.395 for a_p and 7.336 for a_v across all internal
317 pores.



318

319 Fig. 9 (a) Definition of closed pores in digital images. (b) Boxplot illustrating the porosity associated
 320 with open pores and closed pores for tested carbonate sand particles. (c) Slices of the particle skeleton
 321 for a typical particle. (d-e) Visualizations of closed pores and open pores. The colors in the slices
 322 present the pixel of pore regions, and the white color in (d-e) presents the particle skeleton boundary.

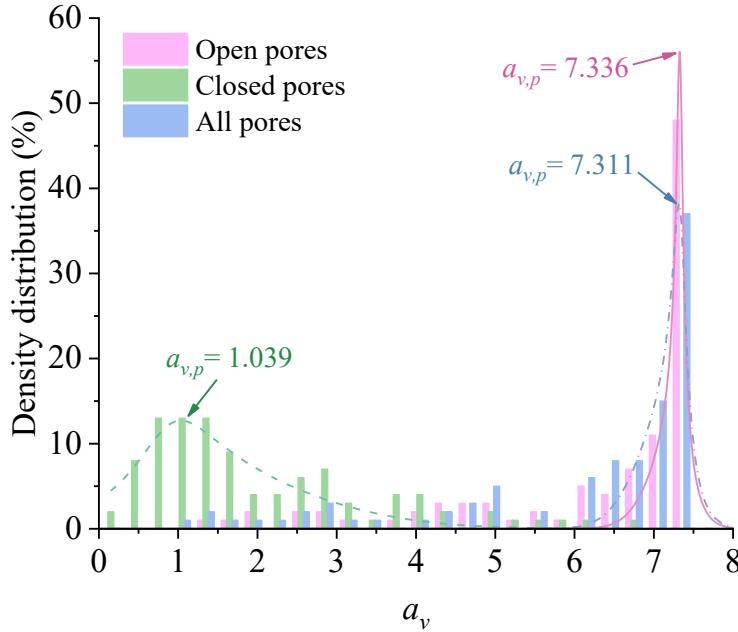
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(a)



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(b)

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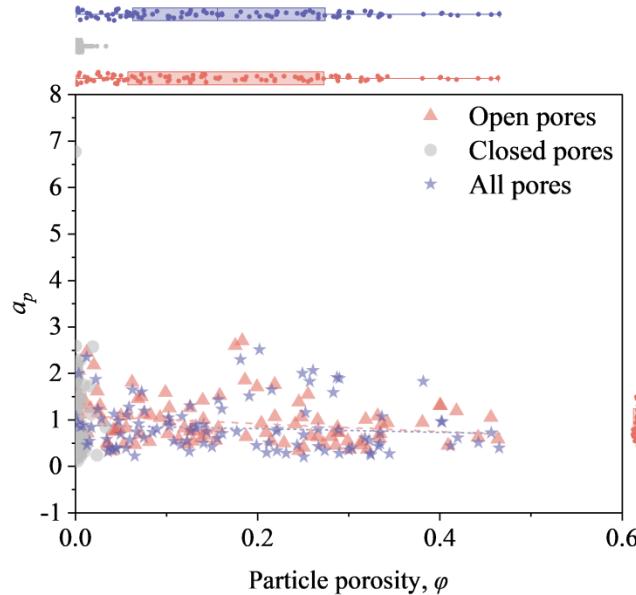
Fig. 10 Variation of (a) a_p and (b) a_v with respect to different pore types

329

330 *4.3 Correlation of pores and particle skeleton parameters*

331 Fig. 11 plots the anisotropy magnitudes against the porosity with respect to different types of
 332 pores. It is observed that the anisotropy parameter a_p does not have a close correlation with the
 333 porosity for both open pores and overall pores. But, a_v for open pores and overall pores exhibits
 334 an increasing trend with the increasing porosity, and eventually converges to a limit value of
 335 7.5 as estimated by Eqs. (7) and (8). This is because the pore network in a particle tends to
 336 exhibit a greater connectivity as the porosity increases, with a good number of relatively small
 337 pores more likely to coalesce into a relatively large pore, rather than remaining individually
 338 isolated. These coalesced large pore structures usually have a greater volume and dominate the
 339 impact on the principal anisotropy direction of the volume-weighted pore orientation vectors.
 340 In this connection, particles with a high porosity (> 0.3) exhibit an extremely high degree of

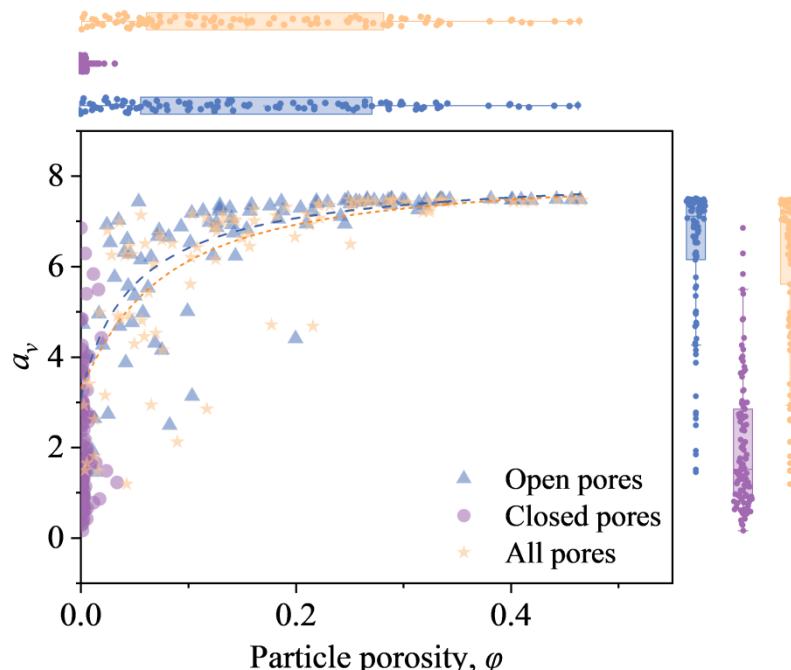
341 volume-weighted pore anisotropy. Additionally, Fig. 11 shows that the variation of anisotropy
 342 magnitudes for the open pores and overall pores are similar to each other, meaning that the
 343 internal pores are primarily composed of open pores, and the closed pores may constitute only
 344 a small fraction of the total pore volume.



345

346

(a)



347

348

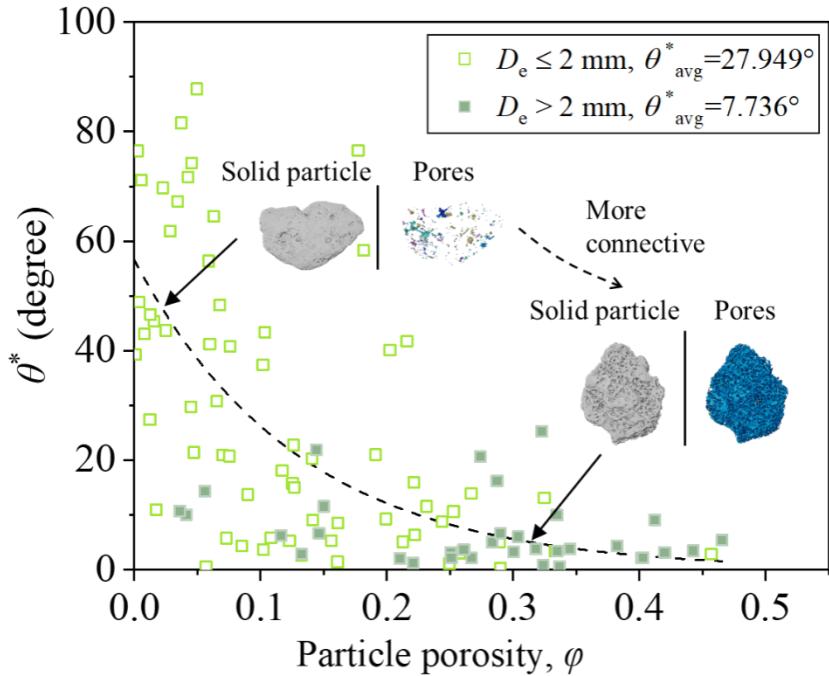
(b)

349

Fig. 11 Variation in anisotropy degrees for different pore types: (a) a_p and (b) a_v

350

351 To probe the correlation between the pore distribution anisotropy and the solid particle
352 skeleton, the angle θ^* , defined as the angle formed between the particle's long axis and the
353 principal anisotropy direction for volume-weighted pore orientation vectors, is plotted against
354 the particle porosity as shown in Fig. 12. It is observed that as the particle porosity increases,
355 θ^* tends to decrease towards zero, with the distribution range narrowing, particularly for the
356 particles with $D_e > 2$ mm. For particles having a low porosity, the pore structure in them may
357 consist of many small pores, resulting in a relatively random pore orientation distribution and
358 a lower anisotropy degree (see Fig. 7). However, for carbonate sand particles of high porosity,
359 a large and highly connected pore structure (depicted in blue) typically dominates the volume
360 of intra-particle pore phase. This large pore structure is an open pore, featuring a large amount
361 of inner channels connected to the exterior surface of particles and exhibiting to some extent
362 the external contour characteristics of the particle's solid skeleton. This has led to a high
363 consistency between the particle orientation and the principal anisotropy direction for the
364 volume-weighted pore orientation vectors.



365

366

Fig. 12 Variation in anisotropy degrees for different pore types: (a) a_p and (b) a_v

367

Various correlation coefficients can be employed to analyze the relationships between

368

parameters, including Pearson and Spearman coefficients. The Spearman rank correlation

369

coefficient effectively characterizes both linear and nonlinear correlations, whereas the Pearson

370

coefficient is only suitable for representing linear correlations. Therefore, the Spearman rank

371

correlation is here used to further analyze the relations of the pore characteristics parameters

372

with the descriptive parameters of particle skeleton morphology, which is expressed as follows

373

$$\rho_{Spearman} = 1 - \frac{6 \sum d_i^2}{n(n^2 - 1)} \quad (11)$$

374

where $\rho_{Spearman}$ is the Spearman rank correlation coefficient, $d_i (= x_i - y_i)$ is the difference between

375

two ranks of each observation, n is the number of observations. The heat map of Spearman

376

correlation coefficients is shown in Fig. 13, where the degree of correlation between two

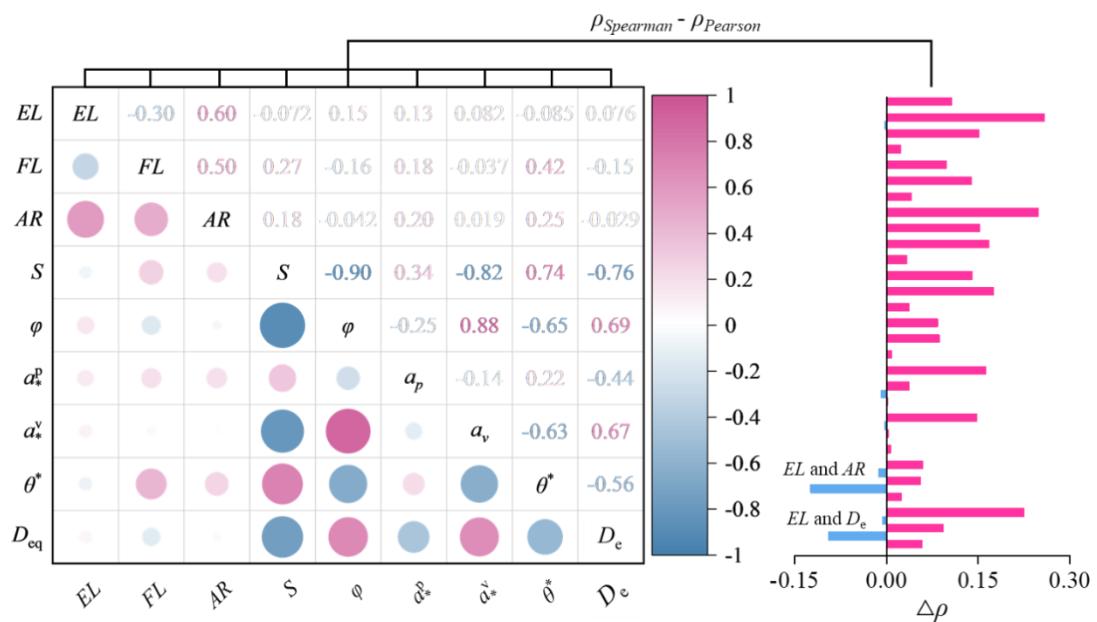
377

characteristic indexes is represented by the red and blue colors in each cell, with red denoting

378

a positive correlation and blue referring to a negative correlation. Notably, a strong positive

379 correlation is observed between the particle porosity and the anisotropy parameter a_v . As both
 380 porosity and a_v increase, the anisotropy parameter θ^* tends to decrease, indicating a complex
 381 interplay between the particle morphology and the anisotropy. Moreover, the sphericity, a key
 382 descriptor of particle shape, shows a significant negative correlation with the porosity and it is
 383 also related to a_v and θ^* , which reveals the connection between the characteristics of the solid
 384 and pore phases in carbonate sand particles. The accompanying bar chart indicates that the
 385 Spearman coefficient is generally higher than the Pearson coefficient for most parameters, with
 386 some exceptional cases such as the coefficient difference between EL and AR . However, it is
 387 important to note that although the anisotropy parameter a_v shows relatively high correlations
 388 with several important parameters, they are not strictly interdependent. This is because a_v is
 389 influenced by the presence of a large and highly connected pore structure in the particle, and
 390 the degree of such correlations depends on the particle size.



391
 392 Fig. 13 Variation of Spearman correlation coefficients between different features

393

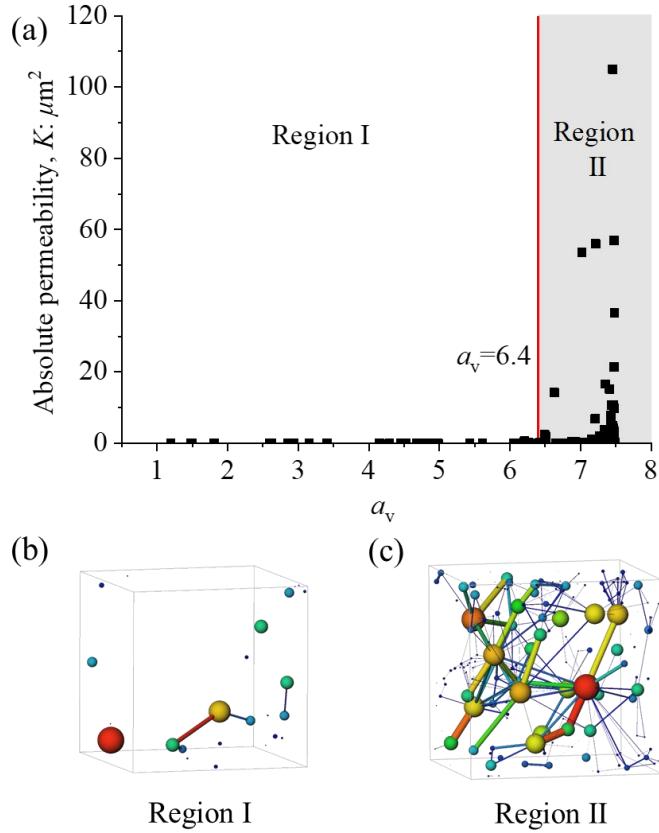
394 4.4 Pore permeability

395 The mechanical behavior of granular assembly depends on the rearrangement of discrete
396 particles in a particular mechanical process, which is accompanied by the variation of inter-
397 particle pores. Also, the permeability of granular assembly is decided by the presence of inter-
398 particle voids. But the influence of intra-particle pores should also not be overlooked, as they
399 affect single-particle properties such as permeability, mechanical strength, and deformation
400 behavior. To further explore this aspect, Fig. 14(a) presents the relationship between a_v and
401 absolute permeability for carbonate sand particles. The permeability of each particle is
402 calculated using the pore network model (PNM) (see Figs. 14b and 14c). The PNM simplifies
403 the complex pore structure into a network of interconnected pores and throats, enabling efficient
404 simulation of fluid flow through porous media. This method has been demonstrated to
405 effectively predict transport properties in previous studies (Zhang et al. 2022; Zhou et al. 2020).
406 In the flow simulation, the input pressure and the output pressure are set at 130 kPa and 100
407 kPa, respectively. The results indicate that for particles with a_v values lower than 6.4, the
408 permeability of particles has minimal influence on the overall fluid transport of an assembly,
409 due to the weak connectivity of internal pores (see Fig. 14b). In contrast, particles with high a_v
410 values (>6.4) exhibit a more interconnected pore network (see Fig. 14c), which facilitates fluid
411 flowing through the particles. In this case, the internal pores would lead to the occurrence of
412 the phenomenon described by Zhou et al. (2023); that is, fluid can permeate the carbonate sand
413 particle even at low seepage pressures. The presence of open pores is found to increase the
414 overall permeability of particle assemblies (Li et al. 2023), and as pore orientation depends on
415 the particle direction (see Fig. 12), variations in particle fabric can introduce complex effects

416 on the fluid transport properties of the assembly.

417

418



419

420 Fig. 14 (a) Relationship between a_v and permeability. (b-c) PNM model for typical carbonate sand
421 particles in different regions. In the PNM, spheres represent individual pores, while sticks represent the
422 throats connecting the pores. The color gradient indicates pore volume, with red denoting larger
423 volumes and blue representing smaller volumes.

424

425 5. Conclusion

426 This study attempts to characterize the spatial distribution of internal pore structures of
427 carbonate sand particles by carrying out the X-ray CT scanning experiments. A vector
428 representation approach is proposed in the framework of statistical micromechanics for the
429 description of pore structures. The major findings are summarized as follows.

430 1. The pore orientation vector, as well as the volume-weighted pore orientation vector,

431 is proposed to describe the spatial distribution of intra-particle pores, and is also used
432 to micromechanically formulate a tensor which characterizes the anisotropic
433 distribution of internal pore structures.

434 2. The anisotropy magnitude of volume-weighted pore orientation vectors is
435 considerably higher than that of pure pore orientation vectors for the carbonate sand
436 particles concerned in this study. For the particles with high porosities, the anisotropic
437 distribution of volume-weighted pore orientation vectors is mainly influenced by the
438 presence of a large open pore that takes up most of the pore space, which makes a_v
439 approximate to the maximum value and principal pore anisotropy direction be close
440 to the particle orientation. For particles with a_v greater than 6.4, the impact of internal
441 pore permeability on the overall hydraulic transport behavior of the particle assembly
442 needs further attention.

443 3. The unique pore structure characteristics of carbonate sand particles exhibit certain
444 relationships with the particle skeleton morphology. However, some correlations,
445 such as those between the sphericity and the porosity and pore anisotropy, are not
446 strictly interdependent, depending on some specific particle characteristics, such as
447 the pore connectivity and size.

448 4. The porosity, pore diameter, and anisotropy parameter a_v all exhibit a dependence on
449 particle size, whereas pore shape parameter (i.e., aspect ratio) does not. The Johnson
450 distribution function is suitable for fitting skewness-kurtosis pore parameter data,
451 while the Gaussian distribution function is more appropriate for symmetrical
452 distributions.

453 **Data Availability Statement**

454 Some or all data, models, or codes that support the findings of this study are available from the
455 corresponding author upon reasonable request.

456

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461

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572

Table 1. Pore characterization parameter distributions using Johnson's fitting method

Distribution parameters	ξ	δ	λ	γ	R^2
Porosity, φ	-0.059	3.712	0.018	-0.887	0.83
Pore orientation anisotropy, a_p	0.377	10.299	0.096	-1.380	0.92
Volume-weighted pore orientation anisotropy, a_v	7.355	13.745	0.089	1.038	0.90