

Article

Multiscale and Fractal Descriptions of Particle Morphology of Calcareous Sand with Different Grain Sizes

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Abstract

The mechanical behavior of calcareous sand differs significantly from that of conventional quartz sands, leading to challenges in offshore geotechnical engineering applications. This distinctive response is closely associated with the complex three-dimensional morphology of calcareous sand particles. However, existing characterization methods are often limited to specific morphological scales and cannot fully describe the multiscale complexity of particle shape. To address this issue, this study performs a comparative morphological analysis of calcareous sand (CS) and Fujian quartz sand (FS) across three particle-size ranges by integrating X-ray micro-computed tomography with spherical harmonic (SH) analysis. Individual particles are reconstructed using SH representation, and a multiscale morphology characterization framework is developed by decomposing particle morphology into three distinct scale levels: large-scale form represented by sphericity, medium-scale angular features represented by roundness, and small-scale surface texture represented by roughness. The results demonstrate that CS and FS exhibit distinct morphological characteristics across different scales, while particle-size effects remain less pronounced within the investigated range. Furthermore, the SH amplitude spectra reveal statistically self-similar characteristics of particle surfaces, allowing the fractal dimension to be correlated with multiscale morphological descriptors. The proposed framework provides a quantitative description of complex particle morphology across multiple scales and may facilitate further investigations of particle-scale mechanical behavior in granular materials.

Keywords: calcareous sand; quartz sand; particle shape; grain size; X-ray

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1. Introduction

Calcareous sand is a special marine biogenic soil, mainly composed of coral fragments, with a calcium carbonate (CaCO_3) content typically exceeding 90% [1–3]. It is widely distributed in tropical and subtropical regions between 30° N and 30° S latitude, as shown in Figure 1. Serving as a primary foundation material for global island and reef engineering, its unique engineering characteristics directly relate to the safety and stability of marine infrastructure [4–6]. Compared with terrigenous sands, calcareous sands exhibit pronounced mechanical peculiarities, including high porosity, elevated compressibility, substantial shear dilatancy, pronounced anisotropy and particle fracturing, which collectively yield responses that frequently diverge from predictions grounded in classical

soil-mechanics frameworks [7–12]. In high-profile projects such as island and reef airports, port facilities, and offshore wind power, the distinctive behavior of calcareous-sand foundations presents a central engineering challenge [13–15].

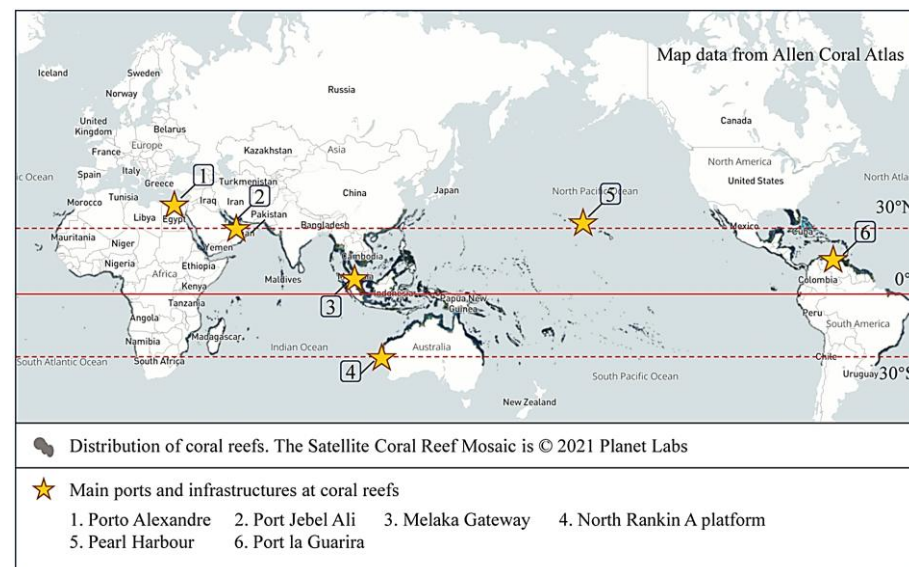


Figure 1. Global distribution of coral reefs and related infrastructures.

Currently, it is increasingly recognized that the above-mentioned macroscopic responses are potentially governed by microscopic geometrical features of individual particles, namely the particle morphology [16–20]. The shape complexity of calcareous sands manifests across scales: at the macroscopic contour level, pronounced irregularity coexists with numerous sharp edges, a combination that frequently promotes particle fracture [21–23]. At finer scales, biological and marine processes may engender even more intricate surface textures [24–26]. This cross-scale morphological heterogeneity far surpasses the descriptive capacity of conventional single indicators based on two-dimensional analysis such as sphericity, aspect ratio and roundness [27–31]. Despite this recognition, the development of a unified three-dimensional geometric description framework capable of quantifying global contour irregularity, local edge sharpness, and surface-texture complexity of calcareous sands remains comparatively limited, partly constrained by experimental capabilities and the lack of a coherent theoretical framework for shape description. Moreover, calcareous sand may exhibit a wide range of size distribution and an unresolved but important question is whether particle shape characteristics systematically vary with size [32–34]. Clarifying these potential relationships could yield insights into the shaping mechanisms of calcareous sand from various sedimentary histories and simultaneously offer guidance for selecting mechanical parameters for calcareous sands across size ranges in engineering practice.

Recent advances in three-dimensional imaging techniques have enabled more comprehensive descriptions of particle morphology. Among these approaches, Fourier-based descriptors have been widely applied to characterize particle boundaries by decomposing surface profiles into frequency components [35,36]. However, most Fourier descriptors were originally developed for two-dimensional contours and are therefore limited in representing complex three-dimensional particle surfaces. Although extensions to three-dimensional Fourier descriptors have been proposed, the interpretation of individual frequency components in relation to specific morphological features remains challenging. Spherical harmonic (SH) analysis provides an alternative framework for representing three-dimensional particle surfaces by decomposing morphology into harmonic components [37,38]. Previous studies have demonstrated its effectiveness in reconstructing par-

ticle shapes and extracting global morphological information. However, existing SH-based approaches mainly focus on shape reconstruction accuracy or overall particle descriptors, while the quantitative interpretation of SH components at different morphological scales remains insufficiently explored. In particular, how harmonic components correspond to different levels of particle morphology, including global form, local angular features, and surface texture, has not been systematically clarified.

With the above considerations, this study aims to address the lack of a unified framework for quantitatively interpreting multiscale three-dimensional particle morphology using SH analysis. Specifically, the morphological characteristics of calcareous sand (CS) and Fujian sand (FS) are systematically investigated across three particle-size ranges using X-ray micro-computed tomography (X-CT) and spherical harmonic (SH) analysis. Based on the analysis of 560 sand particles, the intrinsic evolution of particle morphology during SH reconstruction is systematically examined, and the relationship between SH components and morphological features is quantitatively established. A multiscale reconstruction strategy is then proposed to distinguish particle morphology at three characteristic scales, corresponding to the general form, local angular features, and surface texture. Three scale-specific descriptors—sphericity, roundness, and roughness—are employed to quantitatively characterize the dominant morphological features at each characteristic scale. Subsequently, the multiscale morphological characteristics of CS and FS are compared to evaluate inter-sand differences and particle-size effects. Finally, fractal analysis is integrated with the proposed multiscale characterization framework by establishing the relationship between fractal dimension and multiscale morphological descriptors, providing a comprehensive interpretation of particle morphology across different characteristic scales.

2. Materials and Methodology

2.1. Testing Materials

The calcareous sand (CS) particles analyzed in this study were gathered from an artificial island in the South China Sea [3,39]. CS is predominantly composed of biogenic calcium carbonate, with a specific gravity of 2.69. As shown in Figure 2a, CS particles are characterized by irregular morphologies, including complex shapes, pronounced angularity, and rough surface textures. In contrast, Fujian sand (FS)—presented in Figure 2b—is a natural siliceous sand with a silica content exceeding 98%, consisting mainly of quartz with a specific gravity of 2.65, exhibiting rounded and smooth particle shapes. A total of 280 particles from each sand type were randomly selected, with grain sizes ranging from 0.25 mm to 2 mm, including 100 particles in the 1–2 mm fraction, 100 particles in the 0.5–1 mm fraction, and 80 particles in the 0.25–0.5 mm fraction.

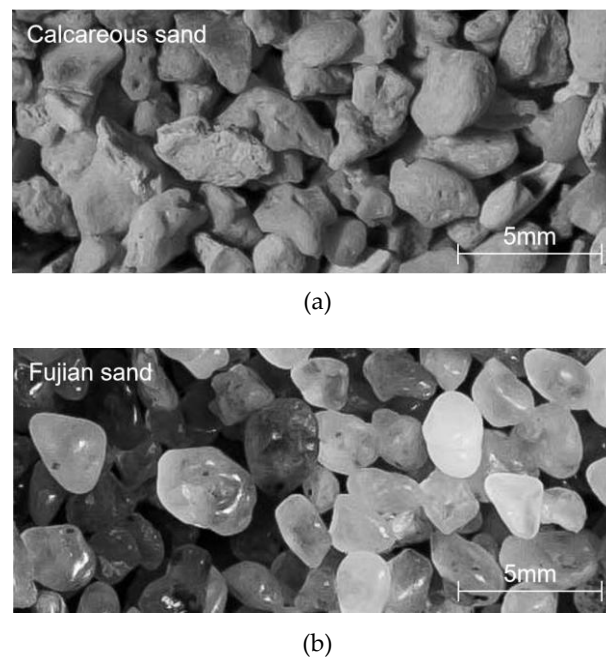


Figure 2. High-definition images of the tested sand: (a) calcareous sand; (b) Fujian sand.

2.2. X-CT Scanning for Sand Particles

To facilitate X-ray micro-computed tomography (X-CT) scanning of individual sand particles, dedicated specimens were prepared in advance to securely immobilize the particles and enhance scanning efficiency and image quality [23,40]. Figure 3 illustrates the preparation procedure of the X-CT scanning specimens. As shown, a two-component fast-curing transparent epoxy resin adhesive was employed to fabricate the scanning samples. The specimen preparation procedure consisted of the following steps: (1) the epoxy resin and curing agent were mixed at a mass ratio of 3:1, thoroughly stirred, and subsequently degassed using a water-bath heating process to remove entrapped air bubbles; (2) the mixture was poured into a mold, after which randomly selected sand particles were immersed in the liquid resin; (3) the particles were arranged sequentially with sufficient spacing between adjacent particles and left to cure at room temperature (25 °C) for 12 h; (4) steps 1–3 were repeated to prepare subsequent layers of the specimen; (5) after completing curing, the specimen was demolded and prepared for X-CT scanning.

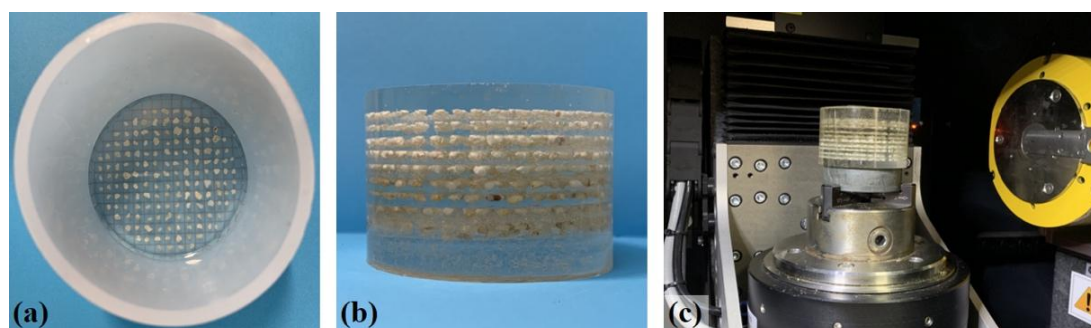


Figure 3. Sample preparation for X-CT scanning: (a) first layer; (b) samples after demolding; (c) X-CT scanning.

An X-ray CT scanner (Phoenix Nanotom S) is used to capture the surface voxel of each particle. To minimize the influence of particle size on the geometric resolution of X-CT images, different voxel resolutions were adopted for different grain-size fractions. Specifically, particles with grain sizes of 1–2 mm, 0.5–1 mm, and 0.25–0.5 mm were scanned

at voxel resolutions of 18 μm , 9 μm , and 4 μm , respectively. This strategy ensured that particles of different sizes were represented with a comparable relative geometric resolution, thereby reducing the potential bias in capturing small-scale surface features caused by differences in particle size. Basic steps and details of X-CT reconstruction are shown in Figure 4. A filter of size 3 is first used to reduce noise in the raw images. Basic steps and details of the X-CT image processing workflow are shown in Figure 4. A filter of size 3 is applied to the raw grayscale images to suppress noise while preserving particle boundaries. The filtered images are then binarized using the Otsu thresholding method, which automatically determines the optimal threshold by maximizing the between-class variance. Since this study focuses on the external morphology of sand particles, the internal pores are filled after segmentation to eliminate their influence on subsequent morphological characterization. The segmented particles are visually inspected to ensure that the extracted boundaries are consistent with the original grayscale images before point-cloud extraction. Finally, the three-dimensional voxel coordinates of each particle are extracted using the Point Cloud plugin in ImageJ (version 1.54i, National Institutes of Health, USA) and are imported into MATLAB R2024a (The MathWorks Inc., Natick, MA, USA), where the particle surface is reconstructed using the Boundary function. The reconstructed voxel coordinates are subsequently used to calculate the particle volume (V), surface area (SA), and the lengths of the three orthogonal axes ($l_a > l_b > l_c$).

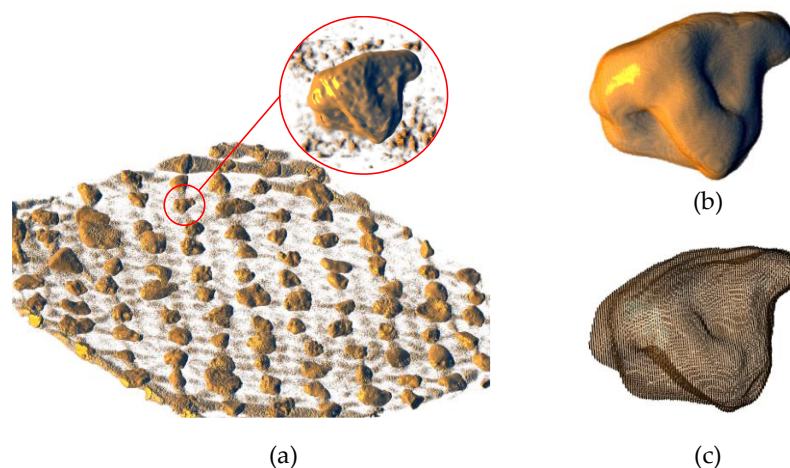


Figure 4. X-CT image processing: (a) image reconstruction of raw slices; (b) image reconstruction of a typical sand particle after segmentation and noise reduction; (c) point data of the particle surface.

According to the classification system proposed by Zingg et al. [41], most CS and FS particles could be considered as “spheroid” when both elongation and flatness are over 2/3, as shown in Figure 5a. Specifically, among the 560 particles analyzed, 326 particles (58.2%) are classified as spheroids, followed by 185 disk-shaped particles (33.0%), 37 rod-shaped particles (6.6%), and 12 blade-shaped particles (2.1%). Furthermore, sphericity S and convexity C are introduced to describe surface compactness of particles [42,43] and their definitions are given as follows:

$$S = \frac{\sqrt[3]{36\pi V^2}}{SA} \quad (1)$$

$$C = \frac{V}{V_c} \quad (2)$$

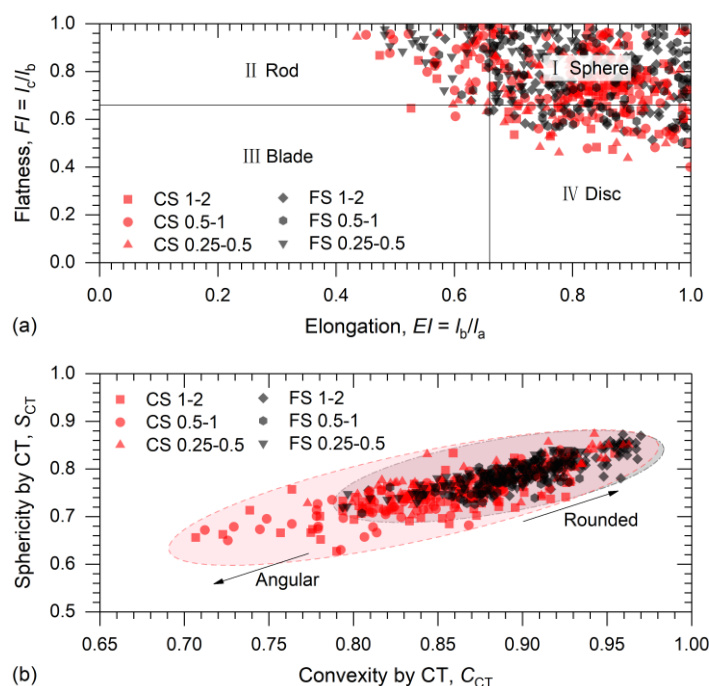


Figure 5. X-CT-based morphological description for CS and FS with different grain sizes: (a) Zingg diagram; (b) convexity versus sphericity.

Where V_c is the volume of the minimum convex boundary of the particle. Sphericity S measures the degree of which an object approaches the shape of its volume-equivalent sphere while convexity C expresses the relative amount that an object differs from a convex object. As shown in Figure 5b, there is a strong correlation between the measured sphericity S and convexity C values, in which values close to 1 represent rounded shapes while smaller values represent angular shapes. It is observed that the distribution of sphericity S and convexity C values of CS is lower and wider than that of FS, indicating that CS particles possess more complex general shapes and richer surface humps. The information obtained from X-CT scanning is an extensive amount of discrete surface point data, requiring a substantial amount of data storage space. The developed particle surfaces are discontinuous and non-differentiable, which is not suitable for detailed morphological examination of complex 3D surfaces [44,45].

2.3. Spherical Harmonic Analysis

To address the limitations associated with X-CT-derived surface data, this study employs spherical harmonic (SH) functions to reconstruct and represent complex three-dimensional particle surfaces. The basic idea of SH analysis is to expand the polar radius of the particle surface from a sphere and use the associated coefficients of the SH series as the mathematical representation of the 3D particle morphology [23,46,47]. The SH formulation can be expressed as follows

$$g(\theta, \varphi) = \sum_{n=0}^{\infty} \sum_{m=-n}^n d_{n,m} u_{n,m}(\theta, \varphi) \quad (3)$$

In this context, $g(\theta, \varphi)$ represents the polar radius measured from the particle centroid, where $\theta \in [0, \pi]$ and $\varphi \in [0, 2\pi]$ denote the spherical coordinate angles. The coefficient of the spherical harmonic series is denoted by $d_{n,m}$. Correspondingly, $u_{n,m}(\theta, \varphi)$ in Equation (3) is expressed as:

$$u_{n,m}(\theta, \varphi) = \sqrt{\frac{(2n+1)(n-m)!}{4\pi(n+m)!}} p_{n,m}(\cos\theta) e^{im\varphi} \quad (4)$$

Here, $p_{n,m}(x)$ denotes the associated Legendre polynomial, which is defined as follows:

$$p_{n,m}(x) = \frac{(-1)^m}{2^n n!} (1-x^2)^{m/2} \frac{d^{n+m}}{dx^{n+m}} (x^2-1)^n \quad (5)$$

In which n and m are the Legendre polynomial's degree and order, respectively. Taking the surface vertex data obtained by X-CT scanning as the input to Equation (3), a set of point data can be simply stored as $(n_{\max} + 1)^2$ SH coefficients. In this paper, the maximum SH degree $n_{\max}$ is set as 15.

A bijective mapping from the surface profile to a unit sphere is created by taking a triangular mapping mesh with 10,240 vertices and 20,480 faces, as shown in Figure 6a, to reconstruct the 3D shell expressed by spherical harmonics. Zhou et al. [45] employed a similar approach for particle morphology reconstruction in their study of Leighton Buzard sand particles and granitic rock outcrops.

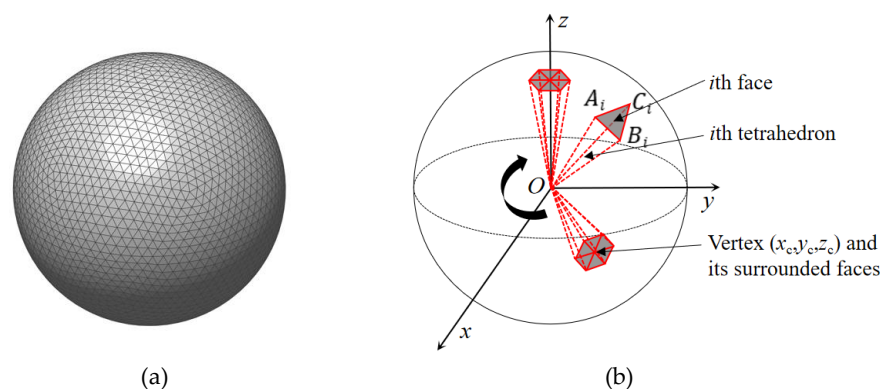


Figure 6. (a) Subdivided-triangular mapping mesh; (b) calculating principles of particle morphological descriptors.

As shown in Figure 7, the SH-based results are in good visual agreement with those obtained from X-CT scanning. In general, in the same size range, CS particles exhibit more irregular shapes, more angular edges, and rougher surface textures than FS particles. Although there are differences in the shape details of different grain sizes for the same type of natural sand, there is considerable similarity in the essential features, such as irregularity, angularity, and rough texture.

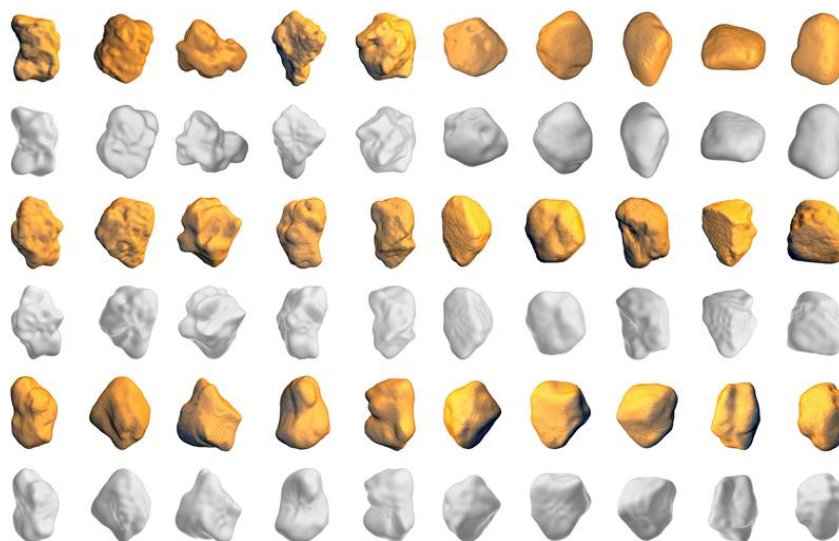


Figure 7. X-CT and SH-based results of typical sand particles with different grain sizes, where the odd rows are X-CT images, and the even rows are SH-based results, while the left five columns are CS, and the right five columns are FS.

To further validate the reconstruction accuracy, the particle volumes obtained from the SH reconstruction at $n_{\max} = 15$ are compared with those measured directly from the X-CT data, as shown in Figure 8. The reconstructed volumes exhibit excellent agreement with the X-CT measurements, with an R^2 value of 0.998 and data points closely distributed around the $y = x$ line, demonstrating the high accuracy of the proposed reconstruction method.

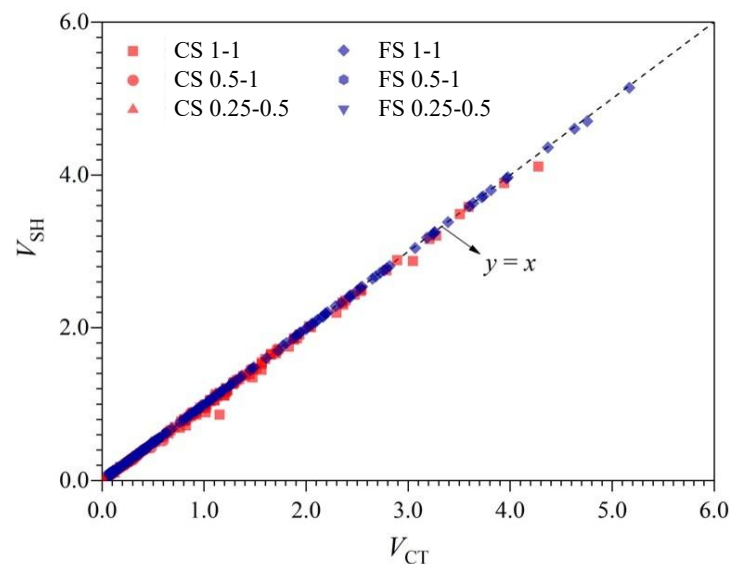


Figure 8. Comparison of particle volumes obtained from X-CT and SH reconstruction at $n_{\max} = 15$.

3. Reconstructed Grain Profiles at Varied SH Degrees

The fundamental concept of SH-based reconstruction of a 3D particle profile relies on the accumulation of harmonic components in terms of A_n defined by SH amplitudes as [48]:

$$A_n = \sqrt{\sum_{m=-n}^n d_{n,m} d_{n,-m}} \quad (6)$$

where $n = 0, 1, \dots, n_{\max}$, and $n_{\max} = 15$. It has been noted that A_1 carries only information on a minor shift in the particle profile relative to the initial location of the particle center and A_0 contains only information on the particle volume [48,49]. Thus, the normalized SH amplitudes A'_n is introduced here as:

$$A'_n = \frac{A_n}{A_0}, \quad n = 2, 3, \dots, 15 \quad (7)$$

This normalized value is used to describe morphology while excluding the influences of particle movement and volume. It is noted that $A'_0 = 1$ represents a sphere of unit volume. In Figure 9, the SH-based morphological components of a representative CS particle at different SH degrees are compared with a standard unit sphere. It is clear that a complete SH-based particle morphology could be divided into fourteen segments of surface fluctuations at different SH degrees. As the SH degree increases from 2 to 15, the value of A'_n decreases and the intensity of the surface fluctuations decreases. From the 2nd to the 4th SH degree, the value of A'_n is reduced from 0.202 to 0.068, which is 22 to 5 times the value of the 15th SH degree (0.009); the corresponding morphological components typically exhibit large surface fluctuations that deviate significantly from the unit sphere. From the 5th to the 8th SH degree, the value of A'_n decreases from 0.047 to 0.022, and the morphological components appear to feature sharp corners and edges on the surface. From the 9th to the 15th SH degree, the value of A'_n converges from 0.018 to a minimum value of 0.009, and the morphological components exhibit densely distributed micro-

humps, forming a rough surface texture. This demonstrates a strong positive correlation between the morphological intensities and the values of A'_n . Hence, morphological characteristics from a large to a small scale level may be mirrored by the normalized SH amplitude A'_n from a low to a high SH degree. More specifically, the morphological components could be classified into three groups according to the amplitudes of variation of A'_n and the intensity of surface fluctuations: the components from the 2nd to the 4th SH degrees $A'_2 \sim A'_4$ characterize the shape features at the large scale-level, the components from the 5th to the 8th SH degrees $A'_5 \sim A'_8$ correspond to the medium scale-level, and the components from the 9th to the 15th SH degrees $A'_9 \sim A'_{15}$ correspond to the small scale-level. The representative CS particle shown here is intended only to illustrate the morphological evolution during SH reconstruction. The proposed three-stage division is established from the statistical analyses of all 560 particles (Figure 10a,b) and is further validated quantitatively by the relationships between normalized SH amplitude and surface fluctuation (Figure 10c).

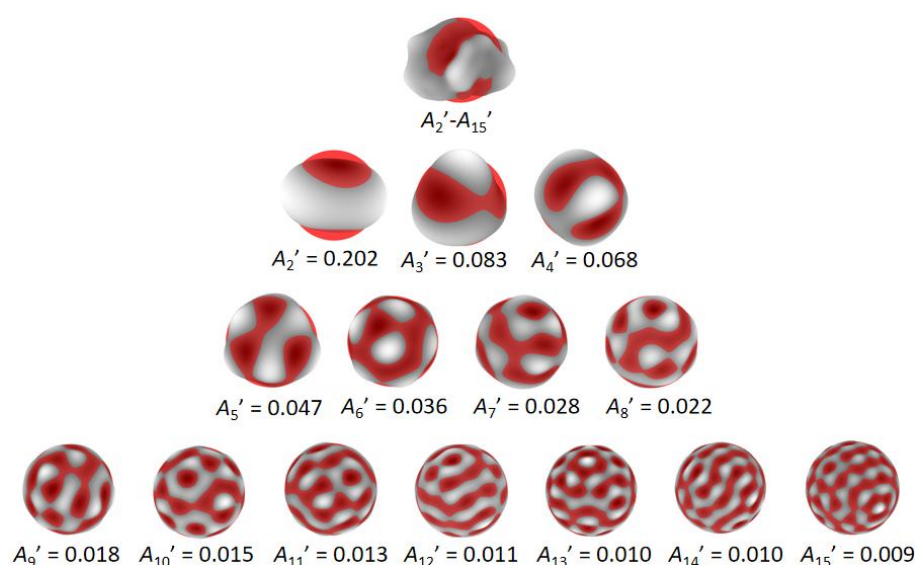


Figure 9. Illustration of the SH reconstruction process using a representative CS particle at different SH degrees, together with its comparison with the red standard sphere at $A'_0 = 1$.

In order to investigate the applicability of this approach, data on 560 CS and FS particles were examined. The intensities of the morphological components were measured quantitatively using the surface fluctuation parameter F_n , which is the ratio of the diameter of the largest inscribed sphere to the diameter of the smallest circumscribed sphere. When the value of F_n increases from 0 to 1, the particle morphology approaches that of a smooth sphere, meaning that the intensity of surface fluctuation weakens and the scale-level shifts from large to small. Figure 10a illustrates the three stages in which the value of A'_n declines as the SH degree increases. The value of A'_n falls rapidly from the 2nd to the 4th SH degree, continues to decline from the 5th to the 8th SH degree, and gradually converges to the minimum value from the 9th to the 15th SH degree. As shown in Figure 10b, the F_n values also experience three stages of change: rapid rise, continuous increase, and convergence. As the SH degree increases, the intensity of the morphological component decreases, indicating subtle surface fluctuations in a lower scale level. The larger scatter observed for the CS particles reflects their greater morphological complexity and natural variability. Nevertheless, the particle morphology is governed by the collective evolution of the complete SH descriptor set rather than by any individual descriptor, and the overall relationships among these descriptors consistently exhibit the same three-stage evolution. Figure 10c provides further confirmation of the strong correlation between A'_n

and F_n , which remains valid for CS and FS particles with various grain sizes and shapes. The greater spread of CS suggests that the morphology of CS particles is more variable and irregular. Toward the direction of smaller A'_n values and larger F_n values, the components are more likely to represent morphologies at lower scale-levels with increasing micro-humps, whereas, in the opposite direction, they are more inclined to characterize morphologies at higher scale-levels with larger surface undulations.

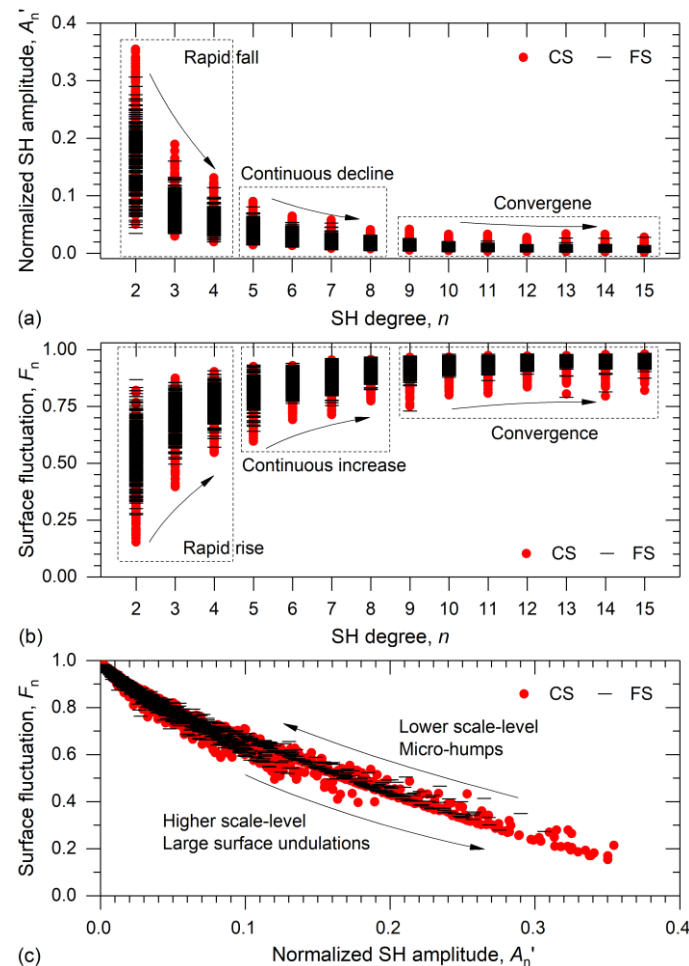


Figure 10. (a) normalized SH amplitude versus SH degree; (b) surface fluctuation versus SH degree; (c) surface fluctuation versus normalized SH amplitude.

4. Multiscale Morphological Descriptions

4.1. A Multiscale Reconstruction Method

Based on the results in Section 3, the normalized SH amplitudes A'_n can be employed to capture and construct particle shapes at definable scale levels. The large scale-level is specifically represented by $A'_2 \sim A'_4$, the medium scale-level by $A'_5 \sim A'_8$, and the small scale-level by $A'_9 \sim A'_{15}$. The division of SH degrees into three characteristic ranges is based on both the visual evolution of reconstructed particle morphology and the statistical evolution of the normalized SH amplitudes obtained from all analyzed particles. As shown in Figure 11a,b, the SH-based full-scale reconstruction replicates the intricate and complex morphological features obtained from X-CT scanning, including the general contour, local boundaries, and surface details. The extracted 3D morphologies, as shown in Figure 11c–e, reflect specific features of the original grain shape at an individual scale level. The large-scale level outlines the general form of the original natural shape, the medium-scale level

describes the local roundness and angles, and the small-scale level characterizes micro-humps and surface texture.

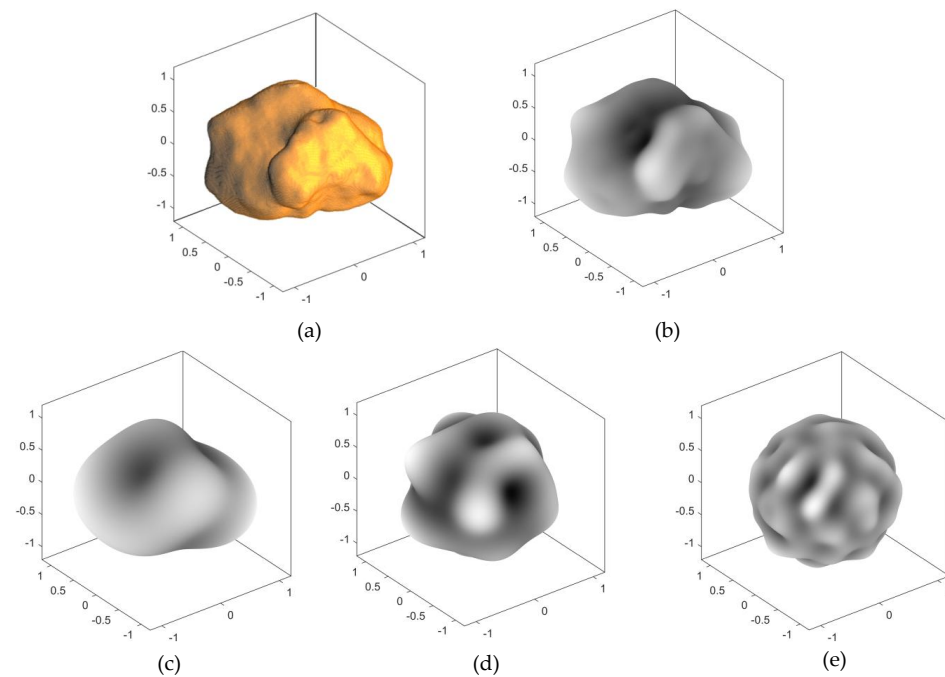


Figure 11. Morphological reconstruction based on scale-level division: (a) X-CT image; (b) SH-based full-scale reconstruction (A_2' – A_{15}'); and morphologies extracted from (c) large-level (A_2' – A_4'); (d) medium-level (A_5' – A_8'); and (e) small-level (A_9' – A_{15}').

4.2. Morphological Descriptors for Each Scale

A number of morphological descriptors may then be defined to identify the features that characterize particle morphology at a certain scale level through explicit SH-based scale-level division and morphological reconstruction. As a result, the naturally intricate and complex particle morphologies can be efficiently separated into distinct scale levels, enabling the determination of morphological parameters corresponding to each scale level. In this paper, three descriptors, i.e., sphericity, roundness, and roughness, are used to quantify particle morphology at three scale levels of general form, local roundness, and surface texture, respectively.

(a) Sphericity S_L

Sphericity S_L uses the same definition of Equation (1), in which the particle volume V and surface area SA are determined by the morphology extracted from the large scale-level ($A_2' \sim A_4'$), is used to express the general form at the large-scale level.

(b) Roundness R_M

In order to characterize local edges and corners of a particle at the medium scale level, roundness is defined as:

$$R_M = \frac{k_{ins}}{N_a} \sum_{n=1}^{N_a} \frac{1}{|k_{n,max}|} \quad (8)$$

where N_a is the number of sharp angles of the particle, k_{ins} is the curvature of the maximum inscribed sphere of the particle, and $k_{n,max}$ is the max curvature of the n -th sharp corners of the particle.

Specifically, the principal curvatures are first calculated for all mesh vertices using the local surface fitting procedure described below. Vertices satisfying $|k_{n,max}|^{-1} \leq R_{ins}$ are identified as sharp corners. For each identified sharp corner, a local micro-surface consisting of the center vertex and its six neighboring vertices (Figure 6b) is extracted. The

maximum principal curvature of the fitted micro-surface is then adopted as $k_{n,\max}$ for calculating the particle roundness.

The micro-surface containing a common center and six edges, as shown in Figure 6b, is analyzed by employing a Taylor series

$$z = g(x, y) \approx a_1 + a_2(x - x_c) + a_3(y - y_c) + a_4(x - x_c)(y - y_c) + a_5(x - x_c)^2 + a_6(y - y_c)^2 \quad (9)$$

where $a_1, a_2, \dots, a_6$ are coefficients to be determined for estimating the local principal curvatures at a specific vertex $v_c(x_c, y_c, z_c)$. Before each computation of the curvature, the micro-surface is rotated to the positive z -axis to overcome the restriction of the Taylor series in the spherical coordinate system. The coordinate set after rotation is given by:

$$\mathbf{v}'_{ms} = \begin{bmatrix} \cos(-\theta_c) \cos(-\varphi_c) & -\cos(-\theta_c) \sin(-\varphi_c) & \sin(-\theta_c) \\ \sin(-\varphi_c) & \cos(-\varphi_c) & 0 \\ -\sin(-\theta_c) \cos(-\varphi_c) & \sin(-\theta_c) \sin(-\varphi_c) & \cos(-\theta_c) \end{bmatrix} \mathbf{v}_{ms} \quad (10)$$

where $\mathbf{v}_{ms}$ and $\mathbf{v}'_{ms}$ are the vectors containing the component vertices of the micro-surface before and after the rotation, respectively, and θ_c and φ_c are the spherical coordinates of the center point. The maximum curvature at an identified vertex can be obtained to describe the nearby roundness of each micro-surface by substituting $\mathbf{v}'_{ms}$ in Equation (10). Equation (9) is then applied to determine the overall roundness of the particle from the morphology extracted from the medium scale-level ($A'_5 \sim A'_8$).

According to Equation (8), R_M theoretically ranges from 0 to 1. A larger R_M indicates smoother and more rounded local edges and corners, whereas a smaller R_M corresponds to sharper and more angular particle morphology. An ideal sphere represents the limiting case of maximum roundness, for which no sharp corners are identified, and Equation (8) is therefore not applicable.

(c) Roughness R_s

It is a common practice to measure the roughness of a fracture surface by comparing its fracture surface area to its projected area on the average topographic plane [50]. Similarly, the surface roughness R_s of a spherical particle in three dimensions could be described by

$$R_s = \frac{SA}{SA_e} \quad (11)$$

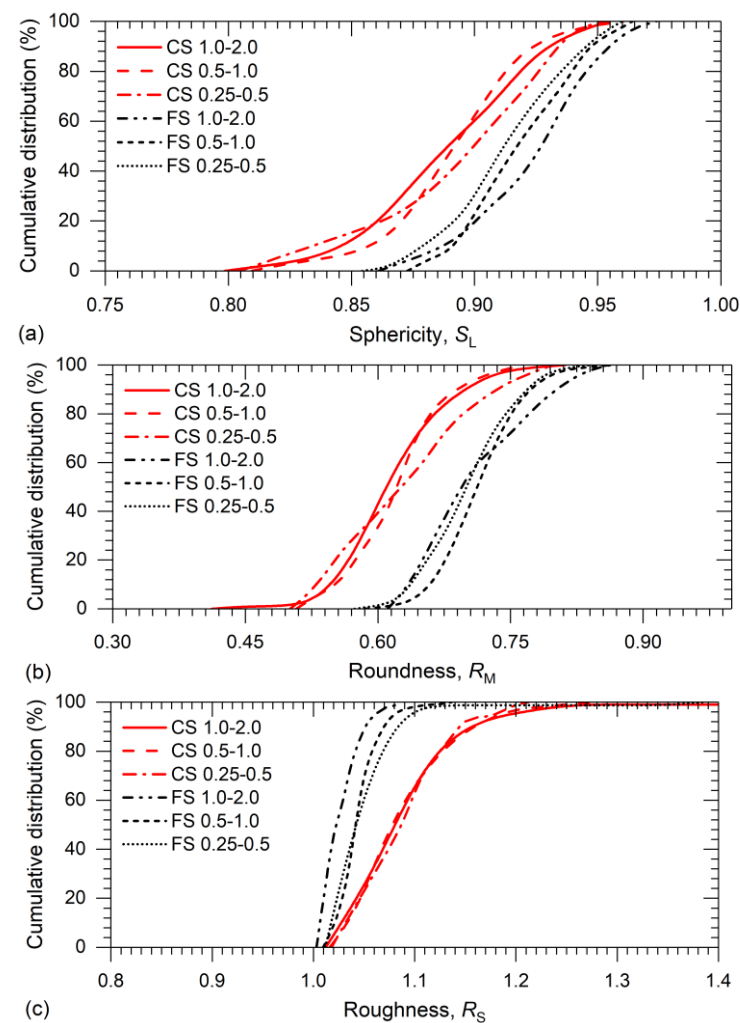
where SA is the surface area of the particle and SA_e is the surface area of the volume-equivalent sphere of the particle. The parameters SA and SA_e are determined by extracting the morphology from the small scale-level ($A'_9 \sim A'_{15}$).

4.3. Comparison Between Calcareous Sand and Quartz Sand

The mean values and standard deviations of the multiscale morphological descriptors are listed in Table 1, and the cumulative distribution functions (CDFs) are shown in Figure 12. It is observed that the distributions of sphericity, roundness, and roughness of the same type of sand with different particle sizes are quite comparable. The maximum sphericity of CS particles is 0.905 for particles in the size range of 0.25~0.5 mm, while the minimum sphericity of CS particles is 0.892 for particles in the size range of 1~2 mm. The average absolute deviation of the sphericity of CS particles is only 0.005. FS has a more rounded general shape as its sphericity (0.915) is 2.0% greater than that of CS (0.897). CS is more angular at the medium scale level, as evidenced by the fact that its roundness (0.628) is 14% lower than that of FS (0.730). The difference in roughness between CS and FS (1.083 vs. 1.023) is 7%, indicating that CS particles are significantly rougher and have more detailed textures. Hence, it may be concluded that the type and origin of natural CS and FS, rather than grain size, determine particle morphology at various scale levels.

Table 1. Multiscale morphological descriptors for CS and FS with different grain sizes.

Sand Type	Grain Size (mm)	Sphericity (S_L)		Roundness (R_M)		Roughness (R_S)	
		Mean Value	Standard Deviation	Mean Value	Standard Deviation	Mean Value	Standard Deviation
CS	1~2	0.892	0.035	0.625	0.062	1.081	0.056
CS	0.5~1	0.894	0.027	0.628	0.053	1.078	0.050
CS	0.25~0.5	0.905	0.036	0.631	0.076	1.089	0.034
FS	1~2	0.921	0.025	0.728	0.072	1.021	0.018
FS	0.5~1	0.914	0.022	0.733	0.053	1.024	0.020
FS	0.25~0.5	0.911	0.024	0.730	0.061	1.025	0.043

**Figure 12.** Cumulative distribution functions (CDFs) of morphological descriptors of (a) sphericity; (b) roundness; and (c) roughness for CS and FS with different grain sizes.

The correlation between any two of the multiscale morphological descriptors is shown in Figure 13. At various scale levels, the correlation patterns of morphological descriptors of CS and FS particles are comparable, although their range distributions are significantly different. The correlation coefficients between sphericity and roundness, sphericity and roughness, and roundness and roughness are 0.676, −0.629, and −0.802, respectively. This demonstrates that the shapes of CS and FS particles exhibit significant self-similarity across multiple morphological scale levels, highlighting the necessity for an effective method to gain insight into this complex feature. These correlations indicate that

particle morphology at different characteristic scales is not randomly organized but exhibits intrinsic geometric relationships. In general, particles with less spherical overall forms tend to possess sharper local edges and more developed surface textures, suggesting that the morphological complexity inherited during particle formation is preserved across scales. It should be noted that the correlation analysis is intended to reveal the intrinsic relationships among the proposed multiscale descriptors. Although CS and FS occupy different value ranges owing to their distinct morphologies, they exhibit similar correlation trends and are therefore analyzed together to illustrate the common multiscale characteristics. Such multiscale relationships provide a useful geometric basis for future investigations into how particle morphology influences the mechanical behavior of granular materials.

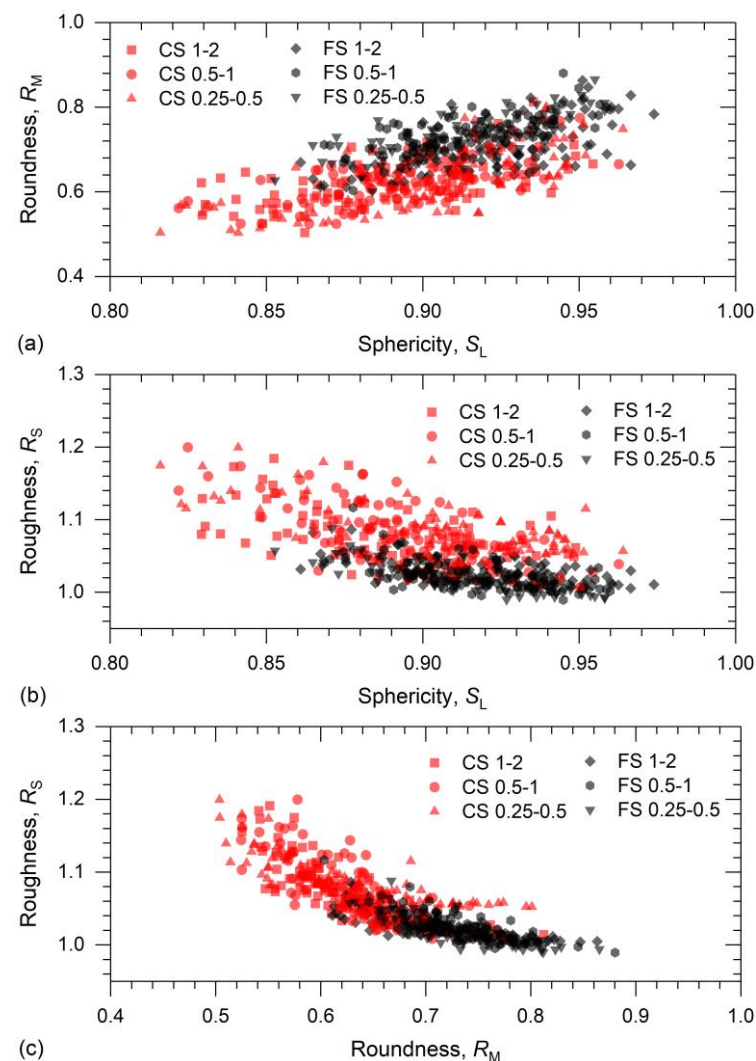


Figure 13. Correlation between the multiscale morphological descriptors: (a) sphericity versus roundness; (b) sphericity versus roughness; (c) roundness versus roughness.

5. Self-Similarity and Fractal Analysis

A self-similar object in geometry refers to an integrated outline that is exactly or approximately identical to one or more of its constituent pieces. Scale invariance is an important property of self-similarity, where the details at an arbitrary scale level are nontrivially similar to the whole [51,52]. A typical example that demonstrates scale invariance is the Koch snowflake [53]. As shown in Figure 14a, as the iteration increases, the fine structures of the snowflake become more complicated and detailed, while remaining to per-

fectly resemble the original form. Similarly, the reconstructed three-dimensional morphologies based on superposition at different ranges of SH degrees also exhibit self-similarity, as shown in Figure 14b. As the SH degree expands to a smaller scale level, details of the particle profile are further increased, but great similarity to the original morphology is always maintained.

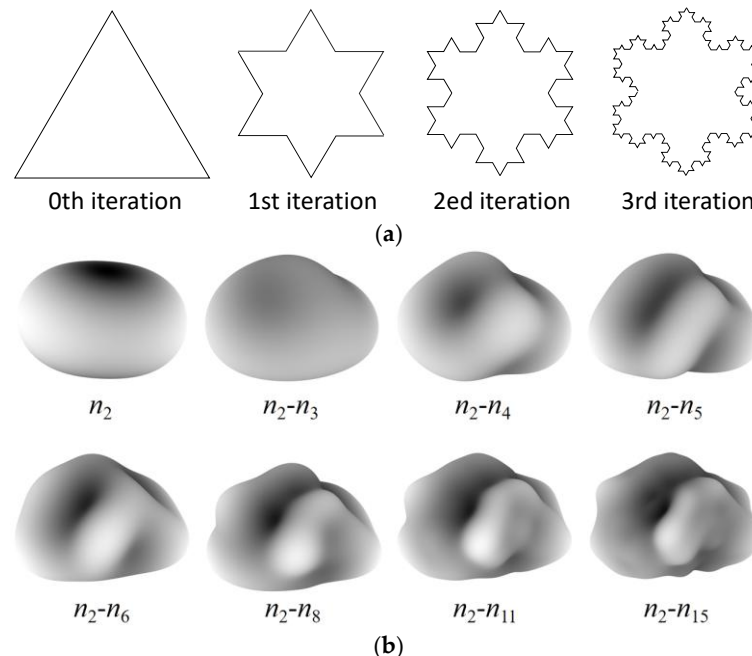


Figure 14. Intuitive morphological self-similarity: (a) typical Koch snowflake as the iteration increases; (b) SH-based morphological superposition as the range of SH degree increases.

Self-similarity is an intrinsic quality of fractals, and the infinite self-similar iterations could be expressed mathematically. Within the framework of fractal theory, a simple geometric measure $M(l)$ evaluated at a characteristic scale l can be expressed as

$$M(l) \propto l^\alpha \quad (12)$$

where α denotes the scaling exponent [54,55]. By taking logarithms, a linear relationship is obtained in log–log space,

$$\log M(l) = \alpha \log l + c \quad (13)$$

where c is a constant.

In fractal analysis, the fractal dimension is determined from the scaling exponent obtained from a power-law relationship in a log–log representation [48]. In this study, the SH amplitude spectrum is used as a scale-dependent description of the particle surface morphology. The harmonic degree n represents different spatial scales of morphological variation, while the normalized SH amplitude A'_n represents the corresponding contribution of each scale. Therefore, the log–log relationship between A'_n and n follows the same scaling principle, and the slope of this relationship provides the scaling exponent α required for estimating the fractal dimension. As shown in Figure 15, for both CS and FS, there is a strong linear relationship between A'_n and n in the log–log scale, and the slope and intercept of the straight line can be easily obtained from linear regression. This is typical for signals with a definable fractal dimension that describes the fractal nature across the multiscale morphological features. The fractal dimension FD is given by

$$FD = 3 + \frac{\alpha}{2} \quad (14)$$

where α is the slope of the regression line of A'_n versus n in the log–log scale.

In Figure 14, it is seen that the mean FD of CS (2.253) is 4% greater than that of FS (2.157), indicating that the particle morphology of CS is more complex and irregular than that of FS across all scale levels. A larger fractal dimension indicates a higher degree of morphological complexity over multiple scales, implying a greater contribution of sharp edges, corners, and fine-scale surface textures to the overall particle geometry. Such geometrically complex particles are expected to exhibit more intricate contact characteristics and stronger interlocking potential, thereby providing a useful geometric basis for interpreting the micromechanical behavior of granular materials.

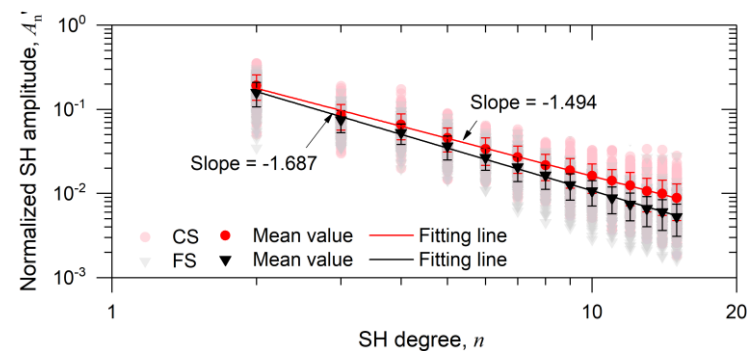


Figure 15. Analytical fractal character: normalized SH amplitude as a function of the SH degree in log-log scales for CS and FS particles.

To evaluate the reasonableness of using fractal dimension for particle morphology characterization, Figure 16 illustrates the correlation between fractal dimension FD and the overall regularity $O_r = (S_L + R_M + 1/R_S)/3$. A strong negative correlation is observed for both types of natural sand, with a correlation coefficient of -0.643 . This relationship indicates that particles with lower overall regularity generally possess greater multiscale morphological complexity, which is consistently captured by a higher fractal dimension. Therefore, the fractal dimension provides an integrated quantitative measure of the combined effects of overall particle form, local angularity, and fine-scale surface texture. This indicates that the multiscale and fractal approaches proposed in this study provide consistent and reliable descriptions of particle morphology. The observed consistency also suggests that fractal dimension can serve as a complementary global descriptor to the proposed multiscale parameters, providing a concise quantitative index for describing the overall complexity of natural particle morphology.

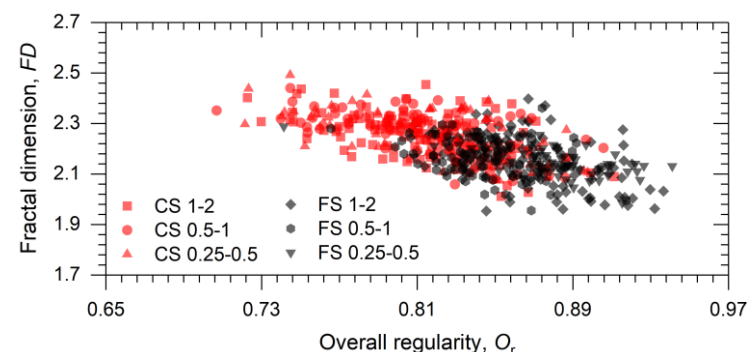


Figure 16. Correlation between overall regularity and fractal dimension for CS and FS with different grain sizes.

6. Conclusions

In this paper, the multiscale and fractal shape features of calcareous sand (CS) and Fujian sand (FS) particles with different grain shapes and sizes are studied based on X-ray

micro-computed tomography (X-CT) scanning and spherical harmonic (SH) analysis. The major conclusions are summarized as follows:

(1) The applicability of spherical harmonics reconstruction for calcareous sand and quartz particles is verified. A strong correlation is observed between the normalized SH amplitudes A'_n and the intensities of surface fluctuations, demonstrating the capability of A'_n to describe multiscale particle morphology. A practical strategy of defining and characterizing particle morphologies from the large, medium, and small scale levels is developed using surface reconstruction. Specifically, particle morphologies at different scale levels are associated with A'_n over distinct ranges of SH degrees: the large scale-level is represented by $A'_2 \sim A'_4$, the medium scale-level by $A'_5 \sim A'_8$, and the small scale-level by $A'_9 \sim A'_{15}$.

(2) Multiscale descriptors of sphericity, roundness, and roughness are proposed to quantify the decoupled morphological features. The results reveal pronounced morphological distinctions between CS and FS, while no consistent size-dependent trend is observed within the investigated particle-size range. These results suggest that, within the investigated particle-size range (0.25–2 mm), particle morphology is more strongly associated with sand type than with grain size. FS has a more rounded general shape as its sphericity (0.915) is 2.0% greater than that of CS (0.897). CS is more angular at the medium scale level, as evidenced by the fact that its roundness (0.628) is 14% lower than that of FS (0.730). The difference in roughness between CS and FS (1.083 vs. 1.023) is 7%, indicating that CS particles are significantly rougher and have more detailed textures.

(3) The strong correlations between the multiscale descriptors suggest significant morphological self-similarity across scale levels for both CS and FS. By constructing three-dimensional morphologies based on spherical harmonic superposition with increasing SH degrees, self-similarity is clearly observed. Increasing SH degrees can be considered as successive magnifications of observation. By continuously zooming to finer scale levels, typical fractal characteristics can be observed. A linear relationship between A'_n and SH degree on a log–log scale confirms the fractal nature of the particle surface and defines its fractal dimension. The mean fractal dimension of CS (2.253) is 4% higher than that of FS (2.157), indicating that the particle morphology of CS is more complex, irregular, and rougher than that of FS across all scale levels. This difference can be attributed to the biogenic origin of calcareous sand, whose coral-derived particles commonly preserve irregular skeletal structures, abundant sharp edges, and intricate surface textures formed during biological growth and subsequent marine weathering processes. This finding aligns with the results of multiscale morphological descriptors.

(4) The proposed multiscale and fractal characterization framework provides a quantitative description of particle morphology across different characteristic scales. The observed weak size dependence within the investigated particle-size range (0.25–2 mm) suggests that representative morphological descriptors may be established according to sand type for the materials considered in this study. The applicability of this conclusion to particle sizes beyond the investigated range requires further investigation. Furthermore, the proposed framework provides a useful basis for future studies on the relationship between multiscale particle morphology and the mechanical behavior of granular materials.

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List of Symbols

Symbol	Definition
V	Particle volume
SA	Particle surface area
SA_e	Surface area of the volume-equivalent sphere
V_c	Volume of the convex hull of the particle
S	Particle sphericity
C	Particle convexity
$g(\theta, \phi)$	Polar radius function of the particle surface
θ, ϕ	Spherical coordinate angles
$d_{n,m}$	Spherical harmonic coefficient of degree (n) and order (m)
$u_{n,m}(\theta, \phi)$	Spherical harmonic basis function
$p_{n,m}(x)$	Associated Legendre polynomial
n	Spherical harmonic degree
m	Spherical harmonic order
$n_{\max}$	Maximum spherical harmonic degree
A_n	Spherical harmonic amplitude at degree (n)
A'_n	Normalized spherical harmonic amplitude
S_L	Sphericity descriptor calculated from large-scale morphology
R_M	Roundness descriptor calculated from medium-scale morphology
R_S	Roughness descriptor calculated from small-scale morphology
k_{ins}	Curvature of the maximum inscribed sphere
$k_{n,\max}$	Maximum curvature of the (n)-th identified sharp corner
N_a	Number of identified sharp corners
R_{ins}	Radius of the largest sphere inscribed in the particle
$v_c(x_c, y_c, z_c)$	Center vertex of the local micro-surface
v_{ms}	Vertex coordinates of the micro-surface before rotation
v'_{ms}	Vertex coordinates of the micro-surface after rotation
$a_1, a_2, \dots, a_6$	Coefficients of the Taylor surface fitting function
O_r	Overall regularity index
$M(l)$	Geometric measure at characteristic scale (l)
l	Characteristic scale
α	Scaling exponent obtained from the log–log relationship
c	Constant term in the log–log scaling relationship
FD	Fractal dimension

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