SCIENCE CHINA
Technological Sciences

February 2013 Vol.56 No.2: 280–285
doi: 10.1007/s11431-012-5094-0

Analysis of the complex morphology of sediment particle surface based on electron microscope images

CHEN ZhiHe[1,2*] & FANG HongWei[3]

[1] *Department of Water Resources and Environment, Geography and Planning School of Sun Yat-sen University, Guangzhou 510275, China;*
[2] *Key Laboratory of Water Cycle and Water Security in Southern China of Guangdong High Education Institute, Guangzhou 510275, China;*
[3] *State Key Laboratory of Hydroscience and Engineering, Tsinghua University, Beijing 100084, China*

Received April 14, 2012; accepted November 22, 2012; published online December 18, 2012

The morphology of sediment particles plays an important role in interfacial interactions. The difficulties in complex morphological description significantly limit the research on interfacial interactions. In this study, images of a single sediment particle extracted from electron microscope photos were used to analyze the gray values and present the probability of shape of the sediment particles. Moreover, the morphological features of the sediment particles were qualitatively described using the fractal method (surface area-volume method). The fractal dimension D of a single sediment particle was calculated to analyze the features and quantitative complexity of the sediment particle morphology. Results indicate that the probability of shape can provide intuitive morphological structure and fully describe the complex morphological characteristics of sediment particle surfaces. The fractal dimension abstractly described the complexity of the morphology of a sediment particle surface and matched well with the experimental results. The methods discussed in this study are suitable for describing the complex morphology of the sediment particle surface and lay the scientific foundation for further research on the interfacial interaction between the sediment particle and the pollutant.

sediment particles, surface morphology, probability of shape, fractal dimension

Citation: Chen Z H, Fang H W. Analysis of the complex morphology of sediment particle surface based on electron microscope images. Sci China Tech Sci, 2013, 56: 280–285, doi: 10.1007/s11431-012-5094-0

1 Introduction

Sediment particles interact with contaminants on the solid-liquid interface of a particle surface. Thus, the morphological structure of sediment particles directly affects surface characteristics and interfacial interactions, thereby affecting the adsorption equilibrium and the combined-state distribution [1–3]. Adsorption of sediment particles not only degrades pollutants in water but also remarkably modifies the surface morphology of sediment particles as a result of substance adsorption and aggregation [4–6]. Reports on the interaction between sediment particles and contaminants are currently available. However, only a few of the studies on interfacial interaction, within the perspective of the morphology of the sediment particles, considered surface structure and characteristics. Studying the interfacial interaction of sediments without describing the surface morphology of the sediment particles is difficult.

The shape factor is often used to represent the deviation of a sediment particle from the standard shape (typically spherical or square). The shape factor is a dimensionless combination of different particle diameters used in many studies to reflect the dynamic characteristics of particles in fluid [7–9]. The shape factor is often used to represent the shape and physical properties of sediment particles in studies on the mechanics of sediment movement because of its versatility and ease of measure [10]. Some researchers

*Corresponding author (email: chzhihe@gmail.com)

compared the different definitions of the shape factor using charts or statistical methods [9, 11–13]. However, this parameter currently has no standard specification.

Quantitative image analysis changes the classification of particle shape based on geometries commonly used in the past. Using graphic processing capability and highly efficient numerical calculation of computers, particle shape can be strictly defined and distinguished to characterize the surface roughness of particles [14–16]. The Fourier Shape Analysis proposed by Schwarcz et al. is the first two-dimensional numerical process that outlines particles. Fractal analysis (first used by Mandelbrot [17]) and fractal harmonics (first discussed by Clark [18]) have been widely used in recent years. Fractal dimension can effectively characterize the roughness of coarse particles, but it cannot provide macroscopic information on particle shape. By contrast, the fractional harmonic function can represent the macroscopic lattice and describe roughness of particles, but its process takes a long time to implement.

Interfacial interactions between sediments and pollutants are related to the surface structure and characteristics of sediment particles. Thus, a research platform that can represent the characteristics of sediments (such as large specific surface area and strong adsorption capacity caused by complex morphology, among others) is urgently needed to improve the description of sediment shape. In this study, the probability of shape was based on the image of a single sediment particle captured using an electron microscope. Gray value statistics were used to describe the shape characteristics of sediment particles. The fractal method (surface area-volume method) was applied to the calculation of the fractal dimensions. The statistical characteristics of the fractal dimensions were analyzed to describe quantitatively the complexity of the sediment particle morphology. The probabilities of sediment particle morphology and fractal dimension, combined with the statistical and fractal methods, were presented to indicate the complex morphological characteristics of sediment particles.

2 Methods

Sand samples were collected from the bed mud in Guanting Reservoir, Beijing. The samples were dried at 105°C for 24 h and then sieved (No. 100 sieve) to remove impurities (such as biological debris) and coarse particles. Electron microscopy and adsorption-desorption experiments were conducted.

2.1 Electron microscopy experiment

Images of a single sediment particle were obtained using a field-emission scanning electron microscope (FESEM, 6301F). The individual sediment particle was the target. The following procedure was used to extract information about the particle of a required size without damaging the images of particles of various sizes obtained using FESEM.

The FESEM images were captured using the unified parameters of the electron microscope to ensure that the images were obtained under the same conditions.

The FESEM images provided the scale, such that the accuracy of the images could be determined using the pixel values within certain scale lengths. For example, a scale length of 10 μm and actual pixel value of 256 became 1 μm = 25.6 pixels after conversion.

Particles with clear boundaries that were easy to recognize and that did not overlap with other particles were separated during particle extraction to ensure unity and integrity.

Figure 1 illustrates the particle images that were extracted from photos obtained using the FESEM. The extracted images were then placed in a pixel frame with a fixed size (e.g., for sediment particles within the size range of 1 μm–5 μm, approximately 5 μm × 5 μm was placed in the extracted particle based on the image scale of 128 × 128 pixel frames). Hence, images of the single particles were obtained as the sample group to study the surface morphology of the sediment particles.

2.2 Adsorption/desorption experiments

The Autosorb-1-C (Quantachrome Instruments) automatic physical and chemical adsorption analyzer was used to measure and investigate the chemical adsorption isotherm and analyze the single-molecule layer cover. This analyzer can analyze fully the pore characteristics on the surface and other physical adsorption characteristics within a measurable range of 0.0005 $m^2\ g^{-1}$–5000 $m^2\ g^{-1}$. Moreover, the Autosorb-1-C analyzer can be used in ultralow-pressure gas adsorption analysis to determine the distribution of micropores and pore sizes with measurable pore sizes of 0.35 nm to 500 nm. Adsorption and desorption curves were plotted according to the FHH fractal theory after the adsorption-desorption experiments. The FHH fractal theory is applicable to the adsorption, desorption, and capillary condensation processes of micropores [19, 20]. The calculations are introduced in Section 2.3.2.

2.3 Fractal dimension of the sediment particle

2.3.1 Fractal dimension of surface morphology

Using image processing and GIS data extraction technolo-

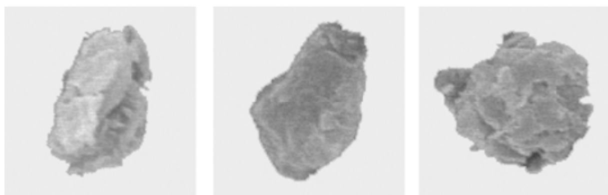

Figure 1 Electron microscope images of individual sediment particles.

gies, the three-dimensional fractal dimensions were obtained by calculating the surface areas and volumes of the particles [21]. The surface area A and volume V for three-dimensional regular figures, such as a ball and cube, among others, exhibit the following relationship:

$$A^{1/2} \propto V^{1/3}. \quad (1)$$

For rough surfaces, such relationship can be extended as follows:

$$\left[A(\varepsilon)/\varepsilon\right]^{1/D} = a_0 \varepsilon^{(2-D)/D} V(\varepsilon)^{1/3}, \quad (2)$$

where a_0 is the curved surface-related constant, D is the fractal dimension, and $A(\varepsilon)$ and $V(\varepsilon)$ are the measured surface area and the volume of the particle at scale ε, respectively. The fractal dimension was $D \cong 2$ when the rough surface was smooth. The logarithm of eq. (2) is expressed as follows to obtain the fractal dimension D:

$$\frac{\log[A(\varepsilon)/\varepsilon^2]}{D} = \log(a_0) + \log\left[\frac{V(\varepsilon)^{1/3}}{\varepsilon}\right]. \quad (3)$$

The diagram of $\log[A(\varepsilon)/\varepsilon^2] - \log[V(\varepsilon)^{1/3}/\varepsilon]$ can be prepared by changing the scale ε. If a linear relationship is obtained, which indicates the fractal characteristics, the slope of the linear portion of the diagram is determined as the value of D.

2.3.2 Fractal dimension of overall morphology

Ref. [22] indicates that pore structures on the surface of sediment particles have fractal characteristics. The overall fractal dimension can be determined using the adsorption-desorption method. The model proposed by Avnir et al. [23] that describes multilayer adsorption on the fractal surface of gas molecules (FHH adsorption model) was used and developed into the following form:

$$N/N_m = k(-\ln x)^{-f(D)}. \quad (4)$$

The linear form is given by

$$\ln(N/N_m) = \ln(k) - f(D)\ln(-\ln x), \quad (5)$$

where $f(D)$ is the function of fractal dimension D, N/N_m is the relative adsorption capacity, x is the relative pressure p/p_0, and k is a constant. The plots of $\ln(N/N_m)$, $\ln[-\ln(p/p_0)]$, and slope $S=-f(D)$ can be generated. Introducing the fractal dimension D to the isotherm equation of Dubinin-Radushkevich for adsorption on porous solid surface, the expression can be rewritten as follows:

$$f(D) = 3 - D. \quad (6)$$

3 Results

3.1 Statistics of the gray values for the morphology of the sediment particle

The surface undulation in the sediment particle image can be reflected by the gray values indicating the differences in the geometric heights of the observed points and their adjacent points. The gray values mirror the relative geometric height of the surface, and the gray value field illustrates the surface topography features. The gray value field can help obtain sufficient information on the surface topography features of the sediment particle [1, 4, 21]. Images of 560 single sediment particles were obtained from the electron microscopy experiment. The image pixel had a 128 × 128 frame. Figure 2 presents the plots of the projected contours at different probabilities. The occurrence probabilities P = 10%, 20%, 30%, ⋯, 90%, and 95% for the enclosed areas are also presented in Figure 2 (from the outside to the inside). The x- and y-axes in the figure indicate the pixel positions. The projected shapes of the sediment particles are demonstrated in Figure 2. Eight observation points along the x- and y-axes were set to analyze the distribution of the gray values. The center of the image was set as observation point O. The gray values of each observation point were obtained to analyze the distribution characteristics of these gray values.

The statistical results of the gray values at different locations in the pixel frame are given in Figure 2 and Table 1. As the observation points approached the center of the pixel frame, the skewness decreased, and kurtosis drastically decreased then increased. For example, the skewness of points 1, 2, and 4 were 3.70, 0.41, and −0.60, respectively. The kurtosis of points 1, 2, and 4 were 15.6, 1.58, and 4.54, respectively. Moreover, the skewness and kurtosis of the central point O were 0.22 and 2.77, respectively. These results indicate that the gray value distribution was slightly skewed. The data contained many values that deviated from the mean value, among which points 1, 8, 9, and 16 were more obvious. The skewness of the statistical results increased because most of the gray values close to the boundary were zero. The statistical results (Table 1) present the non-uniformity of the sediment grain size and the complex morphology characteristics of sediment particles.

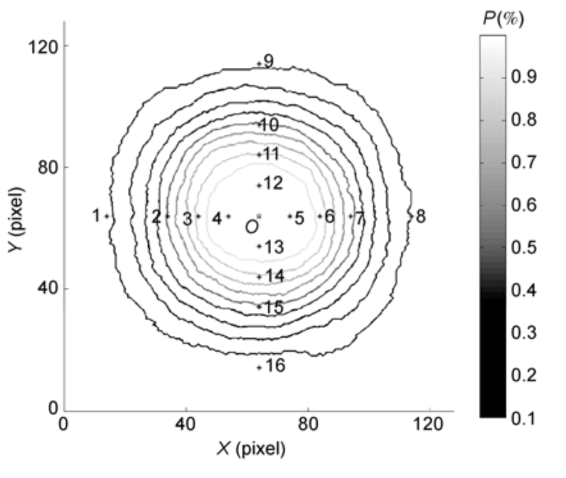

Figure 2 Layout of the sampling points for the statistical analysis of the gray values.

Table 1 Statistical results of the gray values at each observation point

Location	Mean	Standard deviation	Median	Max	Min	Skewness	Kurtosis
1	9.43	34.71	0	203	0	3.70	15.66
2	62.93	68.44	16.5	223	0	0.41	1.58
3	104.25	60.72	119	231	0	−0.63	2.27
4	130.43	38.43	131	248	0	−0.60	4.54
5	126.46	35.34	127	235	0	−0.39	4.62
6	105.99	54.12	116	227	0	−0.75	2.82
7	65.22	66.13	66	240	0	0.28	1.53
8	11.13	37.27	0	195	0	3.37	13.32
9	8.76	32.54	0	186	0	3.80	16.55
10	62.93	68.20	7	223	0	0.38	1.53
11	102.76	60.57	115	224	0	−0.55	2.24
12	130.97	38.36	131	228	0	−0.63	4.82
13	123.31	40.19	123	231	0	−0.64	4.64
14	94.80	60.45	111	231	0	−0.48	2.02
15	54.93	64.20	0	215	0	0.52	1.62
16	5.19	24.90	0	183	0	5.00	27.69
O	132.46	31.82	131	231	45	0.22	2.77

Figure 3 illustrates the reconstruction of the sediment surface at different probabilities. Morphological reconstruction visually expresses the roughness and complexity of a sediment particle surface. The real size of the corresponding particle was 5 μm × 5 μm and 40 nm × 40 nm for the 128 × 128 pixel frame and 1 × 1 pixel grid, respectively. From the perspective of geometry, morphological reconstruction can expand the range from the micron scale of the whole particle to the nanoscale of the particle surface. The statistical results of the surface gray value and the projected shape were directly correlated. The projected shape can reflect the complexity of the surface morphology. However, quantification is limited to the determination of gray values because the projected shape can only indicate relative elevation. Thus, further research is required to improve the results.

3.2 Fractal dimension of the morphological structure of the sediment particle

The surface area-volume method was used to calculate the fractal dimension D for the sample group (Figure 4). The maximum and minimum values of the fractal dimension D were 2.8914 and 2.1557, respectively, the mean and the median were 2.5401 and 2.5439, respectively, the variance and standard deviation were 0.0058 and 0.0764, respectively, and the skewness and kurtosis were −0.18 and 8.12, respectively. These results indicate the concentrated distribution of the fractal dimension D of the sediment particles.

A physical and chemical adsorption analyzer was used according to ref. [22]. Through the adsorption-desorption experiments, and using eqs. (4)–(6), the fractal dimension of the original samples of the sediment particle was calculated to be D_{FHH}=2.7112. The values of D and D_{FHH} were compared and analyzed. Nitrogen molecules fully filled the pores during the adsorption-desorption experiments because of the porous structure of the sediment particle surface. Fractal dimension D_{FHH} describes the complexity of the morphological structure, such that the fractal dimension is $D_{FHH}>D$. The comparative results indicate that the methods applied in this study can quantitatively describe the com-

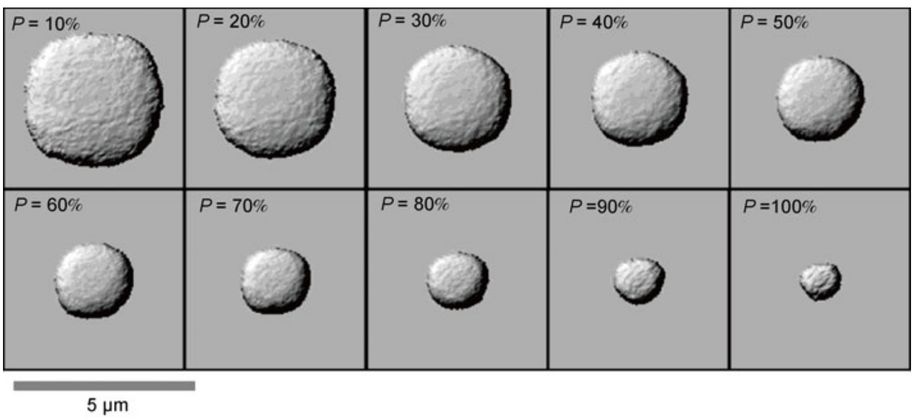

Figure 3 Sediment particle surface at different occurrence probabilities.

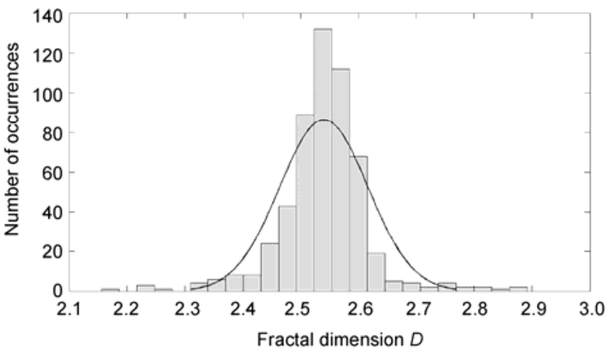

Figure 4 Statistical analysis of the sediment particle *D*.

plexity of the surface morphology of sediment particles.

The morphology of a single sediment particle extracted from the electron microscope image was statistically analyzed. Moreover, the shapes of the sediments with various probabilities and statistical characteristics were presented. The fractal dimension *D* of the morphology of the sediment particle surface describes the complexity of surface morphology. The results matched well with those of the adsorption-desorption experiments, indicating that the methods used in this study are suitable for describing the complex morphology of the sediment particle surface, lay the foundation for research on the interfacial interaction between sediment particles and pollutants, and are advantageous for further research. In addition, sediment settling velocity correction generally adopts the shape factor method without considering the surface roughness of sediment particle [24–26]. This study can be extended to the sediment settling velocity correction in further research, improving sedimentation calculation and sediment transportation simulation accuracy.

4 Conclusions

Images obtained using an electron microscope can provide gray information on the sediment particle surface and demonstrate complex morphologies. Through statistical analysis and fractal qualitative and quantitative studies, the following conclusions were drawn:

(1) The statistical results of the projected shape of the sediment particles indicate that the occurrence probability of gray values can be used to describe the projected shapes of the sample group. Statistical description resulted in better performance in demonstrating the morphological features and the complexity of the sediment particle surface than representation using a single quantitative value.

(2) The complexity of surface morphology can be quantitatively described using the fractal dimension. The fractal dimensions D and D_{FHH} were obtained through the surface-volume method and nitrogen molecule adsorption, respectively. Comparative results indicate that the fractal dimension method is suitable for the quantitative description of the complex morphology of sediment particles.

(3) The probability shape method intuitively provides morphological information on the overall particle and its surface. Fractal dimension abstractly describes the complexity of the morphology of the sediment particle surface. Using the methods discussed in this study, the geometric range of research on particle morphology was extended from the micron scale to the nanoscale.

This work was supported by the National Natural Science Foundation of China (Grant No. 50909107), the China Post-doctoral Science Special Foundation (Grant No. 201003385), and Young Teachers Cultivation Project from Sun Yat-sen University (Grant No. 37000-3161402).

1 Chen Z H, Fang H W, Chen M H. Experimental study on distribution characteristics of copper ions adsorbed on the surface of sediment particles (in Chinese). J Hydr Eng, 2008, 39(5): 633–636
2 Wang Y L, Zhou H W, Yu F L, et al. Fractal adsorption characteristics of complex molecules on particles—A case study of dyes onto granular activated carbon (GAC). Colloids Surf A: Physicochem Eng Aspects, 2007, 299(1-3): 224–231
3 Alberti G, Amendola V, Pesavento M, et al. Beyond the synthesis of novel solid phases: Review on modelling of sorption phenomena. Coord Chem Rev, 2012, 256: 24–45
4 Chen Z H, Fang H W, Chen M H. Simulation analysis on location of copper ion adsorption on sediment particle surface (in Chinese). Adv Water Sci, 2009, 20(1): 69–73
5 Wang Y L, Du B Y, Dou X M, et al. Study on the poresurfacefractal-dimension and surfaceacid–baseproperties of naturalparticlesaround Guantingreservoir. Colloids Surf A: Physicochem Eng Aspects, 2007, 307(1-3): 16–27
6 Fang H W, Chen M H, Chen Z H. Surface pore tension and adsorption characteristics of polluted sediment. Sci China Ser G-Phys Mech Astron, 2008, 51(8): 1022–1028
7 Le Roux J P. A hydrodynamic classification of grain shapes. J Sedim, 2004, 74(1): 135–143
8 Le Roux J P. Grains in motion: A review. Sedim Geol, 2005, 178(3-4): 285–313
9 Blott S J, Pye K. Particle shape: a review and new methods of characterization and classification. Sedimentology, 2008, 55(1): 31–63
10 Göğüş M, İpekçi O N, Kökpinar M A. Effect of particle shape on fall velocity of angular particles. J Hydr Eng, 2001, 27(10): 860–869
11 Bjørk T E, Mair K, Austrheim H. Quantifying granular material and deformation: Advantages of combining grain size, shape, and mineral phase recognition analysis. J Struct Geol, 2009, 31(7): 637–653
12 Jonkers L, Prins M A, Brummer G A, et al. Experimental insights into laser diffraction particle sizing of fine-grained sediments for use in palaeoceanography. Sedimentology, 2009, 56(7): 2192–2206
13 Lira C, Pina P. Automated grain shape measurements applied to beach sands. J Coast Res, 2009, 56(SI): 1527–1531
14 Ahmed M M. Effect of comminution on particle shape and surface roughness and their relation to flotation process. Int J Miner Proc, 2010, 94(3-4): 180–191
15 Greco A, Maffezzoli A. Powder-shape analysis and sintering behavior of high-density polyethylene powders for rotational molding. J Appl Polym Sci, 2004, 92(1): 449–460
16 Hentschel M L, Page N W. Selection of descriptors for particle shape characterization. Particle Particle Syst Char, 2003, 20(1): 25–38
17 Mandelbrot B B. The Fractal Geometry of Nature. San Francisco: Freeman, 1982
18 Clark N N. A new scheme for particle shape characterization based on fractalharmonics and fractal dimensions. Powder Technol, 1987, 51(3): 243–249

19 Grzegorz Józefaciuk A M, Alicja Szatanik-Kloc. Changes of surface, fine pore and variable charge properties of a brown forest soil under various tillage practices. Soil Tillage Res, 2001, 59(3-4): 127–135
20 M Hajnos L K, Pachepsky Y. Soil pore surface properties in managed grasslands. Soil Tillage Res, 2000, 55(1-2): 63–70
21 Wang B J, Shi B, Tang C S. Study on 3D fractal dimension of clayey soil by use of GIS. Chin J Geotech Eng (in Chinese), 2007, 29(2): 309–312
22 Chen Z H, Fang H W, Chen M H. Experiments on fine sediment surface porosity changes after copper ion adsorption (in Chinese). J Sedim Res, 2010(1): 25–29
23 Avnir D, Jaroniec M. An isotherm equation for adsorption on fractal surfaces of heterogeneous porous materials. Langmuir, 1989. 5: 1431–1433
24 Guo J. Logarithmic matching and its applications in computational hydraulics and sediment transport. J Hydr Res, 2002, 40(5): 555–565
25 José A Jiménez, Ole S Madsen. A simple formula to estimate settling velocity of natural sediments. J Waterway Port Coast Ocean Eng, 2003, 129(2): 70–78
26 Benoît C. Simple and general formula for the settling velocity of particles. J Hydr Eng, 2007, 133(2): 229–233