Simulation of sediment particle surface morphology and element distribution by the concept of mathematical sand

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Abstract
Transport of contaminants with sediment is closely connected with the complex surface morphology of particles in the hydro-environment. Based on a large number of experimental results of sediment morphology, we present the concept of mathematical sand which can address the complex surface morphology of suspended sediment. The sand particle can be represented mathematically by a Fourier series that can simulate the shape and size of real particles. The parameters of Fourier series were determined by around 1036 sediment images obtained by a scanning electron microscopy (SEM). Moreover, the distribution of phosphorus on the surface of a mathematical sand particle was proposed based on the statistical results of measured particle’s surface element distribution. The study provided a novel method to explore the relation between the sediment particles and the contaminants.

Keywords: Mathematical sand; SEM; Surface morphology; Element distribution

1. Introduction
Water pollution has become a significant concern in many big rivers of China in the past few decades, including the Yangtze River and the Hai River. As one of the primary carriers, sediment particles play an important role in the transportation and transformation of many contaminants (Darwish, 2013; Pedro et al., 2013). Government officials and environmental researchers have begun to realize the importance of sediments or contaminants in the hydro-environment and have expanded study of the interactions between sediment and contaminants. Much research has focused on the adsorption and desorption kinetics and capacity (Appan and Wang, 2000; Lin and Wu, 2001; Dogan and Alkan, 2003; Jin et al., 2005) and mathematical models for simulating contaminants transport in channels, reservoirs and estuaries (Huang et al., 2007). However, the basic physical and chemical properties of the sediment surface, especially the complex sediment surface morphology, and the interactions occurring at the grain—water interface are still largely unknown. Fang et al. (2008) have conducted preliminary studies of contaminants and their relationship to sediment surface morphology and pore structure. Further work is still needed to make these results more general and useful.

The shapes, roughness and surface textures are so complex that no theory can completely address natural sand particles, as well as the characterization of the ions adsorption to particles. The previously developed models in sediment transportation literature only use the settling velocity and the specific surface area as parameters. As a result, it can hardly represent the complex sediment surface morphology. One of the overall aims of this study is to develop a set of tools that are able to...
describe the ordinary morphology of a sediment particle surface. We would like to present the concept of mathematical sand which can represent the complex surface morphology of the sediment particle. The simulation of mathematical sand was carried out by examining the probability distribution of particle characteristics with different shapes of sediment particle. The element distribution on mathematical sand was subsequently evaluated based on the measured element distribution on real particles. The adsorption and desorption processes are expected to be enhanced by using this mathematical sand model.

2. Descriptions of sediment particle surface

Natural sediment particles were sampled and prepared for image scanning and surface analysis. The particles were sampled at the Yichang hydrology station in Yangtze River, the bottom of Xiaolangdi Reservoir in Yellow River, and the bottom of Guanting Reservoir in Yongding River. These rivers are located in the northern, central and southwestern parts of China, respectively. These particles are much different sizes and the degree of pollution. The median sizes of these particles increase from south to north, as well as the degree of contaminant loading. We have obtained a large number of particle’s images using SEM (see Fang et al., 2013). But it was not easy to obtain the actual three-dimensional particle surface directly, especially for the particles in size less than 0.1 mm. The SEM images of particles provide two kinds of information, the outline of each individual particle and a contrast distribution related to the structure of the particle surfaces. According to the principles of SEM, the contrast gray scale information only shows electron reflections, and does not indicate the actual heights of the particle surface. The outline of each individual particle provides the actual roughness of the particle.

2.1. Analysis of particle outline

MATLAB was used to develop a mathematical model of the particle shapes in SEM particle images. The original images and approximated shapes are shown in Fig. 1. The particle outlines shown in Fig. 1 are closed curves consisting of a series of points. The curve can be represented by a periodic function in polar coordinate.

\[ R(\theta + 2\pi) = R(\theta) \]

where \( R \) is the polar radius and \( \theta \) is the polar angle. The periodic function of the polar radius can be represented by a Fourier series as

\[ R(\theta) = A_0 + \sum_{n=1}^{\infty} [a_n \cos(n\omega\theta) + b_n \sin(n\omega\theta)] \]

where \( n \) is the number of terms in the series; \( \omega \) is frequency (=2\( \pi \)/\( T \), \( T \) is the period); \( A_0, a_n \) and \( b_n \) are the coefficients of the Fourier series which can be calculated using

\[ A_0 = \frac{1}{T} \int_{-\frac{T}{2}}^{\frac{T}{2}} R(\theta) \, dx \]  

\[ a_n = \frac{2}{T} \int_{-\frac{T}{2}}^{\frac{T}{2}} R(\theta) \cos(n\omega\theta) \, dx \]  

\[ b_n = \frac{2}{T} \int_{-\frac{T}{2}}^{\frac{T}{2}} R(\theta) \sin(n\omega\theta) \, dx \]

This Fourier series characterizes the particle’s shape and size. If \( a_n \) and \( b_n \) are zero, the particle is a circular with radius \( A_0 \). Because the size of the selected particles ranges widely, \( A_0, a_n \) and \( b_n \) need to be normalized. If the center is set as original point of a polar system, we can get one \( R_i \) for each \( \theta_i \). Averaging all these \( R_i \) leads to a mean radius \( R_{\text{mean}} \). The resulting coefficients \( A_0, a_n \) and \( b_n \) normalized by mean radius \( R_{\text{mean}} \) thus only characterize particle’s shape. The Fourier series consequently becomes

![Fig. 1. Original SEM particle images and corresponding shapes approximated by MATLAB functions. Top row: original images; Bottom row: approximated shapes. Labels = 2 μm.](image-url)
For a continuous function \( f(x,y) \), the first derivative (gradient) at the point is

\[
\nabla f(x,y) = \left[ G_x \quad G_y \right]^T
\]

where the vector magnitude and direction are

\[
\text{mag}(\nabla f) = \left[ G_x^2 + G_y^2 \right]^{1/2}
\]

\[
\phi(x,y) = \arctan \left( \frac{G_y}{G_x} \right)
\]

The second order derivative is the Laplacian divergence operator, which at point \((x,y)\) is

\[
\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2}
\]

If the particle surface morphology described by the gray scale is continuous, the first and second derivatives can be calculated. Fig. 4 shows the commonly used discrete templates for calculating the first and second derivatives of the gray scale. The first order gradient operator is also called the Sobel operator. The numbers in the box are the relative weights for computing the values at the center point.

The calculated gradient and divergence of the sediment particle surfaces were subsequently transformed into images with pixel values from dark to red. The images are illustrated in Fig. 5. The gradient image shows the various slopes and the variations at the particle edge that can be seen in the original particle, and the divergence image shows the concavity of the surface.

3. Mathematical sand model

Although the gray scale image cannot express the real three-dimensional particle surface directly, it can serve as a foundation for a stochastic mathematical sand model based on the description and analysis of particle shapes (as shown in Fig. 1). Particles were randomly selected for investigation, and a large number of projected particle outlines could be treated as a sample space for outlines. All the outlines projecting from arbitrary viewpoints of all particles form a whole space. When the number of observed particles is sufficiently large, the distribution of the sample space can be used to evaluate the distribution of the whole space. As a result, an outline, produced by a sufficiently robust sample space, can be regarded as a stochastic outline of a sediment particle.

Among the three sediment samples, we gained more images for the particles from the Guanting Reservoir because we were more concerned about the fine particles located there. The statistical analysis was based on around 1036 SEM images for sediment particles from Guanting Reservoir. Since most of the \( d_{50} \) of suspended load in Chinese rivers is typically between 0.002 mm and 0.03 mm, the sample particles were divided into three groups, \( d_{50} < 0.015 \text{ mm}; 0.015 \text{ mm} < d_{50} < 0.04 \text{ mm}; d_{50} > 0.04 \text{ mm} \), respectively. Table 1 provides the numerical characteristics of coefficients of Fourier series in Equation (4).

Fig. 2. Comparisons between natural particle shape and predicted particle shape using the Fourier series. (a) \( n = 10, R^2 = 0.9669 \); (b) \( n = 20, R^2 = 0.9795 \). \( n \) is the number of terms of Fourier series. Triangles: points on the edge; Solid line: Fourier fitting.

\[
R_s(\theta) = A_{i0} + \sum_{n=1}^{N} \left[ a_{sn} \cos(n\theta) + b_{sn} \sin(n\theta) \right]
\]

where \( A_{i0} = A_0/R_{\text{mean}}; a_{sn} \) and \( b_{sn} \) are normalized coefficients of the Fourier series.

The more terms in the Fourier series are evaluated, the better the representation of the particle surface is. Fig. 2(a) and (b) compares the outline of a typical particle with the curve fit predicted using Equation (4) with 10 and 20 terms. It can be seen that the model accurately predicts the actual particle shape with a sufficient number of coefficients \( a_{sn} \) and \( b_{sn} \). Fig. 3 illustrates the relationship between the correlation coefficient \( R_s^2 \) and number of terms \( n \). It shows that the shape prediction is satisfactory when \( n \) approaches to 10 and that is used herein.

2.2. Analysis of surface relative height

The SEM also provides gray scale images as shown in the figures. Although the gray scale does not indicate the actual heights along the particle surface, the first derivative of the gray scale can be used to represent the surface slopes while the second derivative represents the degree of pitting.
The variation of each coefficient is quite different, but no causation between them was found by further analysis (data not shown).

Fig. 6 shows the probability box plot of $a_m$ and $b_m$, in which the symbol $-$ denotes maximum and minimum value, symbol $\times$ denotes 10% and 90% position of the values, symbol $\perp$ denotes 25% and 75% position of the values, symbol $\circ$ denotes averaged value, and the line position in the closed zone denotes medium value. This plot depicts the distribution of each coefficient. Some of the terms have a larger range than others.

The stochastic function of sediment surface morphology is assumed to follow a normal probability distribution $N(\mu, \sigma^2)$. For the defined significance level $\alpha$, there is a sample $(X_1, X_2, X_3, \ldots, X_n)$ whose average value $\bar{x}$ and standard deviation $s$ are used to estimate the confidence interval of population mean $\mu$ and variance $\sigma^2$. The confidence interval of population mean $\mu$ and variance $\sigma^2$ can be calculated by the data of average value and standard deviation from Table 1 using interval estimate method. The results are shown in Table 2. It can be seen from the table that the probability distribution of coefficients of Fourier series overall follows a normal probability distribution, and satisfies population mean and variance of 95% degree of confidence. It shows that the parameter characteristics of this sample can be regarded as the parameter characteristics of the population.

Since these coefficients are normalized and only characterize the particle’s shape, they can represent the shapes of many other river sediment samples. The statistical distributions for $a_m$ and $b_m$ thus can be used to mathematically model sediment particle shapes. Random outlines can be produced by randomly selecting $a_m$ and $b_m$ which follow a given Gaussian distribution. These outlines are subsequently assembled as planes into a three-dimensional mathematical sand model.

The model particle is reconstructed by using 180 planes with only 1° interval and specifying the origin of the coordinates at the center of the “sphere” (see Fig. 7). The coordinate of each mesh point on the surface can be calculated by the latitude and longitude of the point. It can be seen from the figure that there are many depressions and asperities on the surface, which can represent the natural sediment particle surface morphology. In addition, the precision of the mathematical model relies on the SEM resolution. For example, for a 128 pixels by 128 pixels SEM image of a 4 µm x 4 µm particle, the precision of the mathematical model is 30–40 nm. Thus, the reconstruction only represents the primary structural information of the particle’s fluctuant surface without micro-pores. Higher resolution SEM images will give better mathematical models.

The mathematical sand discussed herein is primarily utilized to describe contaminant fate in the area of hydro-environment, so the topography variation of its surface is especially important. In order to verify the reliability of the mathematical sand model, two integrated indexes, fractal dimension (FD) and specific surface area (SSA), were used to compare the mathematical sands with the real sand. The FD and SSA for real sediment particles were measured by nitrogen adsorption experiments. The values of FD and SSA for particles from Guanting Reservoir whose size ranges from 0.002 mm to 0.029 mm are 2.5854 and 59.87 m² g⁻¹, respectively (Chen, 2008). The FD for mathematical sand particle was calculated by the length–area–volume relations (Mandelbrot, 1983). The SSA for mathematical sand particle was directly calculated from its definition. The calculated FA and SSA for a mathematical sand particle who has the same medium size as the real particles from Guanting Reservoir are 2.5559 and 60.123 m² g⁻¹, respectively. The errors of these two indexes are only 1.14% and 0.4%, respectively. The comparison shows that the mathematical sand model presented above can represent the surface complexity of real sediment particles.

4. Phosphorus distribution on model particle

It is difficult to measure the dynamic process of adsorption and desorption on a microscopic scale. However, the interaction of adsorption and desorption processes can be deduced from equilibrium experiments. Batch isotherm adsorptions can evaluate contaminant sorption capacity and lead to observation of elemental distribution on the surface under an equilibrium
condition. The results of the elemental distribution on the natural particle surface can subsequently be extended to the mathematical sand because the mathematical sand model has a statistical characteristics equivalent to that of natural sand particles.

Once we obtained the model particle, we could calculate the coordinates of all mesh points on the surface as previously stated. Each point on the surface and their eight surrounding points form a micro-surface (also called micro-structure) which is assumed to be local, smooth and continuous and can be mathematically described by a polynomial equation. The definitions in topography, such as peak, ridge and pit, can be mathematically described by a polynomial equation, which is assumed to be local, smooth and continuous and points form a micro-surface (also called micro-structure) stated. Each point on the surface and their eight surrounding particles.

\[ C_u = \frac{1}{2} (C_{\text{max}} - C_{\text{min}}) \]  

wherein \( C_{\text{max}} \) and \( C_{\text{min}} \) are maximum and minimum profile convexity, respectively (Chern and Osserman, 1975).

Fang et al. (2013) conducted batch P sorption experiments on sediment particles from Guanting Reservoir and measured the elemental distribution maps of adsorbed particles using Energy Dispersive X-ray Spectroscopy (EDS). The spectroscopy can output a map of specified element distribution (P in our research) on a certain area of a particle’s surface, e.g. 4 µm × 4 µm, thus the numbers of specified element atoms or function groups can be counted. The distribution map can be projected to the corresponding particle surface obtained simultaneously. Thus, the phosphorus distribution was linked with the surface morphology. Similarly, the geometric quantities (e.g. \( C_{\text{max}} \) and \( C_{\text{min}} \)) of the surface micro-structure can also be calculated. The calculation is based on SEM images of the particle captured by a scanning electronic microscopy. The images are gray pictures and consist of several grid shaped pixels. The difference between gray values of image pixels indicates relative height difference on the particle surface while the difference between elevations of a model particle is the actual height difference. The gray values were previously scaled by the \( d_{50} \) of the particle. Through this linkage between element distribution map and particle surface morphology, the experiment gave a result that the relation between non-spherical curvature \( C_u \) and the amount of P adsorption which can be expressed as an exponential function (Fang et al., 2013),

### Table 1
Numerical characteristics of the coefficients of Fourier series.

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Min</th>
<th>Max</th>
<th>Mean</th>
<th>Std err.</th>
<th>Max err.</th>
<th>Sq err.</th>
<th>Skewness</th>
<th>Kurtosis</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a_{11} )</td>
<td>−1.910</td>
<td>1.934</td>
<td>−0.004</td>
<td>0.398</td>
<td>3.844</td>
<td>0.158</td>
<td>−0.289</td>
<td>14.331</td>
</tr>
<tr>
<td>( a_{12} )</td>
<td>−0.236</td>
<td>1.547</td>
<td>0.007</td>
<td>0.090</td>
<td>1.783</td>
<td>0.008</td>
<td>11.937</td>
<td>193.779</td>
</tr>
<tr>
<td>( a_{13} )</td>
<td>−1.167</td>
<td>10.673</td>
<td>0.014</td>
<td>0.567</td>
<td>11.841</td>
<td>0.322</td>
<td>14.212</td>
<td>267.414</td>
</tr>
<tr>
<td>( a_{14} )</td>
<td>−1.016</td>
<td>17.134</td>
<td>0.038</td>
<td>0.799</td>
<td>18.150</td>
<td>0.638</td>
<td>20.925</td>
<td>448.469</td>
</tr>
<tr>
<td>( a_{15} )</td>
<td>−1.303</td>
<td>12.635</td>
<td>0.035</td>
<td>0.615</td>
<td>13.938</td>
<td>0.378</td>
<td>18.329</td>
<td>376.630</td>
</tr>
<tr>
<td>( a_{16} )</td>
<td>−1.417</td>
<td>1.123</td>
<td>0.006</td>
<td>0.235</td>
<td>2.540</td>
<td>0.055</td>
<td>−0.172</td>
<td>16.255</td>
</tr>
<tr>
<td>( a_{17} )</td>
<td>−12.179</td>
<td>1.052</td>
<td>−0.022</td>
<td>0.599</td>
<td>13.231</td>
<td>0.358</td>
<td>−17.862</td>
<td>363.805</td>
</tr>
<tr>
<td>( a_{18} )</td>
<td>−16.003</td>
<td>0.719</td>
<td>−0.030</td>
<td>0.750</td>
<td>16.722</td>
<td>0.563</td>
<td>−20.593</td>
<td>439.061</td>
</tr>
<tr>
<td>( a_{19} )</td>
<td>−10.253</td>
<td>0.526</td>
<td>−0.016</td>
<td>0.479</td>
<td>10.779</td>
<td>0.230</td>
<td>−20.778</td>
<td>444.444</td>
</tr>
<tr>
<td>( a_{20} )</td>
<td>−1.709</td>
<td>0.521</td>
<td>0.001</td>
<td>0.099</td>
<td>2.230</td>
<td>0.010</td>
<td>−10.247</td>
<td>194.840</td>
</tr>
<tr>
<td>( b_{11} )</td>
<td>−1.178</td>
<td>7.246</td>
<td>0.025</td>
<td>0.422</td>
<td>8.424</td>
<td>0.178</td>
<td>10.625</td>
<td>184.415</td>
</tr>
<tr>
<td>( b_{12} )</td>
<td>−0.150</td>
<td>2.077</td>
<td>0.008</td>
<td>0.115</td>
<td>2.227</td>
<td>0.013</td>
<td>13.856</td>
<td>235.890</td>
</tr>
<tr>
<td>( b_{13} )</td>
<td>−1.865</td>
<td>5.884</td>
<td>0.020</td>
<td>0.494</td>
<td>7.748</td>
<td>0.244</td>
<td>3.382</td>
<td>47.422</td>
</tr>
<tr>
<td>( b_{14} )</td>
<td>−3.225</td>
<td>1.882</td>
<td>0.008</td>
<td>0.419</td>
<td>5.107</td>
<td>0.176</td>
<td>−0.763</td>
<td>18.738</td>
</tr>
<tr>
<td>( b_{15} )</td>
<td>−15.716</td>
<td>1.347</td>
<td>−0.028</td>
<td>0.781</td>
<td>17.063</td>
<td>0.609</td>
<td>−17.316</td>
<td>349.053</td>
</tr>
<tr>
<td>( b_{16} )</td>
<td>−21.045</td>
<td>0.797</td>
<td>−0.038</td>
<td>0.984</td>
<td>21.842</td>
<td>0.968</td>
<td>−20.762</td>
<td>443.770</td>
</tr>
<tr>
<td>( b_{17} )</td>
<td>−15.071</td>
<td>0.705</td>
<td>−0.026</td>
<td>0.701</td>
<td>15.776</td>
<td>0.492</td>
<td>−21.071</td>
<td>452.691</td>
</tr>
<tr>
<td>( b_{18} )</td>
<td>−3.108</td>
<td>0.853</td>
<td>0.001</td>
<td>0.181</td>
<td>3.960</td>
<td>0.033</td>
<td>−10.547</td>
<td>190.151</td>
</tr>
<tr>
<td>( b_{19} )</td>
<td>−0.462</td>
<td>6.221</td>
<td>0.019</td>
<td>0.303</td>
<td>6.683</td>
<td>0.002</td>
<td>18.326</td>
<td>375.281</td>
</tr>
<tr>
<td>( b_{20} )</td>
<td>−0.292</td>
<td>6.935</td>
<td>0.019</td>
<td>0.328</td>
<td>7.226</td>
<td>0.108</td>
<td>20.030</td>
<td>422.509</td>
</tr>
</tbody>
</table>
\[ N_i = 0.77e^{-0.68C_u} - 0.82e^{-1.27C_u} \]  

(10)

where \( N_i \) is the total number of P adsorbed on all micro-surfaces with \( C_u \); \( N \) is the total number of P adsorbed on the whole particle surface.

Since we obtained the \( C_u \) value of each micro-surface belonging to the model particle surface and the relation between \( C_u \) values and P sorption for the actual sediment particle, we can distribute P to the mathematical sand surface. We assume the same P distribution law between model and actual particle.

Batch sorption experiments on target sample are used to obtain the maximum P sorption capacity and to relate this to \( N \). The bonding energy constant with the Langmuir isotherm model can be represented by Stumm (1992) and Huang et al. (1995),

\[ X = \frac{X_mKC}{1 + KC} \]  

(11)

where \( X \) is the amount of adsorbed P on unit mass of particles (mg/g); \( X_m \) is the maximum adsorption capacity of unit mass of particles (mg/g); \( C \) is the water phase equilibrium concentration (mg/L) and \( K \) is the binding energy constant. The amount of P adsorbed on unit mass of particles, \( X \), under a certain equilibrium P concentration can then be calculated using Equation (11) when \( X_m \) and \( K \) are already known. Subsequently, \( N \) can be calculated as

\[ N = \left[ \frac{X \cdot m_0}{m_p} \right] \]  

(12)

where \( m_0 = 1/6\pi r_s d_{50}^2 \) is the mass of one mathematical sand particle with \( R_{\text{mean}} = d_{50} \) and \( r_s = 2650 \text{ kg/m}^3 \); \( m_p = 5.149 \times 10^{-20} \text{ mg} \) is the mass of one phosphorus atom.

The total number of P adsorbed on all micro-surfaces with \( C_u \) can then be calculated using Equation (10). One \( N_i \) corresponds to a \( C_u \). There are many micro-surfaces having the value of \( C_u \), but not every micro-surface has a chance to adsorb a P. So the P is randomly distributed to the micro-surfaces that have \( C_u \) assuming a uniform distribution law. Each micro-surface has two states having or not having a P. Fig. 8 shows the calculated P distribution on the surface of a model particle. Red points represent phosphorus at the grid point of model particle.

5. Discussions

Sediment particle surface morphology affects phosphorus adsorption onto particles. The goal of the mathematical model particle is to represent the complexity of the surface, not only the surface morphology but also the surface pores, and thus represent P sorption.

5.1. The impact of surface morphology on adsorption

The complexity of the particle surface morphology contributes to the differences of lattice structure between mineral components and other precipitates. The heterogeneity of lattice structure leads to variations in surface charge which affects the interactions between mineral and contaminant on the water–sediment interface (Huang et al., 2012). Different kinds of surface morphology and lattice structure have different binding energies, so they have different rate and stability for P sorption.

We developed two ways to describe the surface morphology. One is to classify the micro-structures using geography concept. Six micro-structures (peak, ridge, channel, pass, pit and slope) are defined (Fang et al., 2013). The numbers of P adsorbed on these micro-structures can be counted and analyzed after we capture the SEM image and P mapping. The P distribution on the model particle is related to those same micro-structures. The other approach is to calculate the non-spherical curvature on each local micro-surface. The distribution law stated previously, an exponential function, shows a single-peak skew distribution in a normal coordinates system. To eliminate the influence of particle size on non-spherical curvature and improve the applicability, all curvature values were normalized. The statistical data is
plotted in Fig. 9, and following a log normal distribution. This distribution law can also be applied on our model particle. With the increase of curvature on the surface, the probability of adsorption of phosphate ions increases at first, and then decreases based on the distribution. For another model particle, the distribution of adsorption sites differs due to redistribution of surface morphology but using the same distribution law.

5.2. The impact of surface pores on adsorption

Previous studies on adsorption kinetics indicated that both physical adsorption and chemical adsorption coexist in contaminant adsorption processes (Tinsley, 1979; Lin and Wu, 2001; Dogan and Alkan, 2003). In the early stage of adsorption, contaminants, such as phosphate ions, are rapidly attracted to particle surface under the action of van der Waals forces. These contaminants, however, would desorb into solution by the actions of flow shear stress because this physical adsorption is reversible. Subsequently, the contaminants diffuse from the solution into the surface pores because of the capillary action of pores. Since the shear stress is much smaller in the surface pores, contaminants there are more stable and remain absorbed. The results of experiment on clean sediment and their adsorption of P show that the averaged pore size and total surface pore volume of particles decrease after the particles adsorbed phosphate (Fang et al., 2008). The surface pores thus play an important part in the interactions between sediment and contaminants.

Scanning electronic microscopy has not yet advanced to allow capture of the smallest pores on the particle surface. So the mathematical particle model based on particle profiles analysis cannot represent the impact of these pores yet. The resolution of mathematical model particle developed in this paper is about 30–40 nm, but the normal size of micro-pores on sediment surface is about 2–10 nm. New microscopy

Table 2
Confidence interval of population mean and variance, when degree of confidence $\alpha = 0.05$.

<table>
<thead>
<tr>
<th>Coefficients</th>
<th>Mean</th>
<th>Lower confidence limits</th>
<th>Upper confidence limits</th>
<th>Sq. err.</th>
<th>Lower confidence limits</th>
<th>Upper confidence limits</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_{11}$</td>
<td>-0.004</td>
<td>-0.040</td>
<td>0.032</td>
<td>0.398</td>
<td>0.374</td>
<td>0.425</td>
</tr>
<tr>
<td>$a_{12}$</td>
<td>0.007</td>
<td>-0.001</td>
<td>0.015</td>
<td>0.090</td>
<td>0.084</td>
<td>0.096</td>
</tr>
<tr>
<td>$a_{13}$</td>
<td>0.014</td>
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Fig. 7. A three-dimensional mathematical sand model representing particle surface morphology with a variety of slopes and indentations.

Fig. 8. P distributions on a model particle. Red points represent phosphorus at the grid point of model particle. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
devices with higher resolution should be used to obtain the specific information of surface pores. This is what we would mainly focus on in near future. In addition sediment with different properties of surface morphology and surface pores, such as kaolinite and montmorillonite, also requires study.

6. Conclusions

(1) The Fourier series can comprehensively describe the complexity of sediment particle outlines and reconstruct the mathematical sand which made us be able to study the relation between particle surfaces and interfacial interactions such as sorption and desorption. (2) The measured FD and SSA of real sediment particles from Guanting Reservoir whose size ranges from 0.002 mm to 0.029 mm are 2.5854 and 59.87 m² g⁻¹ while those of mathematical sand having same medium size are 2.5559 and 60.123 m² g⁻¹, respectively. The small errors show that the mathematical sand model can represent the surface complexity of real sediment particles. (3) The sediment particle surface morphology strongly affects the distribution of P adsorbed onto particles. Statistical analysis shows that the relation between non-spherical curvature and the amount of P adsorption can be expressed as an exponential function which could be extended to mathematical sand. (4) The micro- and macro-pores on the particle surface will be the main focus of our future work. Observation and measurement will be downscaled to nano-dimensions. Meanwhile, sediment with different properties of surface morphology and surface pores, such as kaolinite and montmorillonite, should also be studied separately.

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References