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Research paper

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

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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.

$$R(\theta + 2\pi) = R(\theta) \tag{1}$$

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

$$R(\theta) = A_0 + \sum_{n=1}^{\infty}[a_n \cos(n\omega\theta) + b_n \sin(n\omega\theta)] \tag{2}$$

where n is the number of terms in the series; ω 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

$$A_0 = \frac{1}{T}\int_{-\frac{T}{2}}^{\frac{T}{2}} R(\theta)\mathrm{d}x \tag{3a}$$

$$a_n = \frac{2}{T}\int_{-\frac{T}{2}}^{\frac{T}{2}} R(\theta)\cos(n\omega\theta)\mathrm{d}x \tag{3b}$$

$$b_n = \frac{2}{T}\int_{-\frac{T}{2}}^{\frac{T}{2}} R(\theta)\sin(n\omega\theta)\mathrm{d}x \tag{3c}$$

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 θ_i. Averaging all these R_i leads to a mean radius R_{mean}. The resulting coefficients A_0, a_n and b_n normalized by mean radius R_{mean} thus only characterize particle's shape. The Fourier series consequently becomes

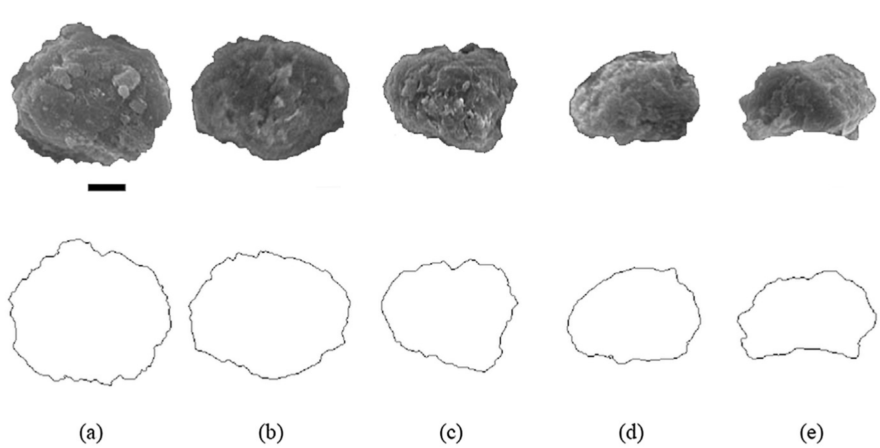

Fig. 1. Original SEM particle images and corresponding shapes approximated by MATLAB functions. Top row: original images; Bottom row: approximated shapes. Labels = 2 μm.