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Reconstruction of multiphase microstructure based on statistical descriptors

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HIGHLIGHTS

- We describe the two-point correlation function of multiphase microstructure.
- We discuss the lineal-path function of multiphase microstructure.
- The procedure of simulated annealing for multiphase microstructure is discussed.
- We show that the reconstructions can capture the main property of the original image.
- Different sections of the 3D generation reflect the similarity and variability in real sandstone.

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ABSTRACT

The microscopic structural features of porous media directly affect their macroscopic properties (e.g., mechanical, electromagnetic, capillary, and transport properties). As for sandstone, the distributions of the clay and the pore in three-dimensional (3D) space have important effects on its electrical conductivity and transport property. In this paper, the experiment of the two-dimensional (2D) and 3D reconstructions of multiphase microstructure (pore, grain, and clay) based on 2D images was carried out. In the reconstruction procedure of simulated annealing for multiphase microstructure, three independent two-point correlation functions and two lineal-path functions are chosen as the morphological information descriptors. Another important morphological descriptor of microstructure is the two-point cluster function, which is used to validate the reconstruction results. From the result of the 2D reconstruction, it is found that the 2D generation is similar with the original 2D image in morphological information and their correlation functions match very well, which illustrate that the presented method has the ability to generate the 2D microstructure from the original 2D image for multiphase microstructure. In the case of 3D reconstruction, the two-point correlation functions and lineal-path functions of the 3D generation are in excellent agreement with that of the original 2D image, and comparison of the two-point cluster functions from the slices of the 3D generation with the original image reflects the similarity and the variability of the slices in real sandstone, which illustrate that the presented methodology is effective and proper for the reconstruction of 3D microstructure based on the 2D image.

1. Introduction

Porous media, which is commonly existence in natural and man-made materials, is composed of solid material skeletons and many crowded tiny pores created by the partition of material skeletons [1–8]. In porous media, the effective properties

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(e.g., mechanical, electromagnetic, capillary, and transport properties) are determined by their complex microstructures (e.g., the volume fraction, morphology, and spatial distribution of components). To quantitatively understand the microstructure – property relationship in porous media, there is a need to obtain the real three-dimensional (3D) structure of porous media. In many cases, it is difficult to obtain the real 3D structure of porous media [9]; only a two-dimensional (2D) image is available. In this case, reconstructing 3D microstructure based on a 2D image is the fundamental method of reproducing the geometry and spatial distribution of components. An effective reconstruction procedure enables one to generate accurate structures and subsequent analysis can be performed on the 3D structure to obtain the desired macroscopic properties of the media.

There are numbers of approaches that have been taken to reconstruct the random media [10–24]. A widely adopted reconstruction method is based on the statistical feature functions, which is also called statistical correlation functions [15–24]. Two general approaches based on statistical reconstruction have been actively pursued in recent years. The first method is based on the conditioning and truncation of Gaussian random fields: successively passing a normalized uncorrelated random Gaussian field through a linear and then a nonlinear filter to yield the discrete values representing the phases of the structure [15–19]. This approach is mathematically elegant and computationally very efficient but model dependent, as it cannot impose constraints other than the volume fraction and the two-point probability function in the reconstruction process. This is a serious drawback.

Another popular approach of statistical reconstruction is the simulated annealing (SA) algorithm [20–31]. This approach is model independent and, in principle, it can include any type and number of statistical correlation functions as constraints to reproduce the morphological information. Moreover, this method is applicable to multidimensional and multiphase media. This method was first introduced by Torquato and Yeong in 1998 [13], which starts with a given, arbitrarily chosen, initial configuration of a random medium and a set of target functions. The target functions describe the desirable statistical properties of the porous media of interest, which can be various correlation functions. This method can be seen as finding a realization (configuration) making the discrepancies between the statistical properties of the realization and that of the original 2D structure minimized. By interchanging the phases of pixels in the digitized system, the target functions are gradually approaching the minimization, which illustrates that the reconstruction owns the similar distribution with the original structure.

The microstructure of porous media contains complex spatial structure information, which can be characterized by different types of statistical descriptors. Different statistical functions contain distinctive morphological information. In general, a single lower-order function cannot fully represent a structure. To overcome the weaknesses of individual statistic functions and to make use of the useful information included in each statistic function, an arbitrary number of different correlation functions can be accommodated in the reconstruction process. Reservoir sandstone is commonly composed of multiple components (phases) and the distributions of the clay and the pore in 3D space have important effects on its electrical conductivity and transport property. To clarify and quantify the relationships between the microstructure and macroscopic properties, reconstructing the 3D microstructure based on 2D image is needed. Some researchers have conducted some research on this problem [32–39]. In this paper, the SA method was chosen to reconstruct multiphase microstructure. In the reconstruction process, multiple statistic functions (both two-point correlation function (TPCF) and lineal-path function (LPF)) are used as constraints to reproduce the complex spatial structure information.

The outline of the rest of the paper is as follows: In Section 2, the basic distribution functions as the morphological information of multiphase porous media are described. In Section 3, the reconstruction method for digitized media, which utilizes both TPCFs and LPFs as statistical descriptors, is briefly outlined. In Section 4, the reconstruction of multiphase microstructure is discussed. It is noted that the presented method can capture the salient properties of the original structure, which can be used to analyze its macroscopic properties [40–42]. Finally, the concluding remarks are made in Section 5.

2. The description of the morphological information

2.1. Two-point correlation function

TPCF is calculated by throwing a number of random vectors on the microstructure [3], depending on the likelihood of the beginning and end of each vector ($\vec{r}$) lying in a particular phase and examining the number fraction of the sets (vectors) which satisfy the different phases (Fig. 1(a)). For a two-phase microstructure, there are only two phases, phase 1 and phase 2, with the volume fraction of each phase defined as

$$\frac{V_k}{V_{total}} = \upsilon_k, \quad k \in [1, 2], \tag{1}$$

where V_1 and V_2 are the volumes of the two phases, respectively, and υ_1 and υ_2 are their corresponding volume fractions. Clearly,

$$\sum_{k=1}^{2} V_k = V_{tot} \quad \text{and} \quad \sum_{k=1}^{2} \upsilon_k = 1. \tag{2}$$