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3D Stochastic Replicas of Porous Solids: A Way to Improve Predicted Diffusivity

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1. Introduction

Theoretical evaluation of diffusivity and permeability of porous media requires a quantitative description of their microstructure, particularly geometry and topology of pore space. Three-dimensional stochastic reconstruction based on statistical information extracted from images of two-dimensional cuts through porous media offers an interesting way to model the microstructure. The extracted statistical information is usually expressed in the form of selected microstructural (morphological) descriptors that are common for two-dimensional and three-dimensional representations of porous media [1]. Liang et al. [2] showed that stochastic reconstruction constrained by low-order statistical information (e.g. total porosity and the two-point probability function) can result in marked differences in geometry and connectivity, which correlated with differences in specific surface area. Therefore, we focused our attention on processing digital images that would provide low-order statistical information conforming to another independent measurement. Specifically, specific surface area derived from the two-point probability function should conform to specific surface area determined using the BET method.

2. Description of methodology

Three samples of macroporous bodies, which were manufactured by pressing fused alumina grains and a ceramic binder, and which differed in total porosity and mean pore sizes, were investigated. Series of back-scatter electron images of cross-sections were recorded with an appropriate size and resolution.

Raw images that were slightly imbued with noise were filtered and segmented. Nonlinear filters, explicitly the median filter and the alpha-trimmed mean filter with masks of different shapes and sizes, were applied to suppress noise and to smooth pore walls. Segmentation using a global threshold assigned black or white to each pixel in an image. As a result, binary images, in which each pixel represented either the void phase or the solid phase, were created. Finally, the binary images were treated using a filter with an adaptive neighbourhood. This filter selectively removed small clusters of pixels and preserved complexity of pore walls. Its parameter defined a size of the largest clusters that was removed from an image. A key problem of image processing and analysis related to 3D stochastic reconstruction is a choice of its parameters, values of which are often arbitrary. We suggested a method of estimating image processing parameters. In our method the parameters were iteratively adjusted so that calculated total porosity and specific surface area would be close to their counterparts obtained from helium pycnometry,

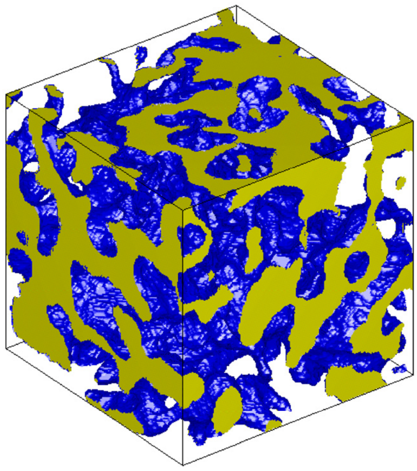

Fig. 1. 3D stochastic replica shown as a subregion of 160×160×160 voxels. Pore orifices are yellow, pore-solid interface is blue, and solid matrix is transparent.

mercury porosimetry and low-temperature adsorption of krypton. We also investigated the influence of the image processing parameters on the courses of the two-point probability function, lineal-path function and two-point cluster function. These descriptors were used in our modified method of stochastic reconstruction using simulated annealing [3]. An example of obtained replicas is shown in Fig. 1.

3. Conclusion

Our careful treatment of back-scatter electron images of polished sections enabled specific surface area derived from the two-point probability function to conform to its counterpart derived from the BET measurement. Thus, representative models of the real porous media reconstructed by our method will be used as a starting point to simulate gas diffusivity. The simulation results will be compared to diffusivity of replicas reconstructed using the two-point probability function whose slope at the origin will not correspond with experimental specific surface area.

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