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3D stochastic replicas of porous solids: A way to improve predicted diffusivity

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Abstract

The goal of our contribution was to develop a method providing morphological (microstructural) descriptors whose values would match total porosity and specific surface obtained other independent methods. The model obtained from limited amount of statistical information, accessible by image analysis of cross-sections, offers an attractive way for the prediction of equilibrium and transport phenomena in natural and man-made macroporous media.
Key words: transport phenomena, morphological descriptors, image processing, segmentation.

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 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. Experimental

Three samples of macroporous bodies, which were manufactured by pressing fused alumina grains of various sizes and a ceramic binder, and which differed in total porosity and mean pore sizes, were investigated. Cylindrical pellets of size 5×5 mm were made of abrasive corundum grains and a binder (Electrite, a.s., Benátky nad Jizerou, Czech Republic). Their basic properties were estimated using standard methods of textural analysis, i.e. mercury intrusion and helium density measurement. All macroporous materials exhibit monodisperse pore-size distributions differing in the most frequent pore diameters, see the following Table 1.

Table 1. The properties of the investigated samples of porous material.

Material label	A	B	C
Specific surface, μm^{-1}	0.031	0.052	0.057
Total porosity	0.322	0.292	0.308
Pore diameter[a], μm	38.0	18.1	13.5

[a] It denotes the most frequent pore diameter derived from mercury porosimetry.

After drying, these pellets were impregnated with epoxy resin Araldite® under vacuum. Hardened epoxy resin blocks were cut, ground, and polished to achieve the smooth surface. Series of 2D backscatter electron (BSE) images (40–60 images) were recorded with an appropriate size (1280 × 960) pixels and resolution. The grey intensity of each pixel in an image represents the atomic numbers of elements prevailing in the area which a narrow beam of electrons is focused on. The higher the atomic number, the brighter the pixel appears, i.e. pores filled by the epoxy resin are black or dark grey.

3. Image processing and image analysis

Raw images (Fig. 1 left) that were slightly imbued with noise were filtered and segmented (Fig. 1 right). Non-linear filters, explicitly the median filter and the α-trimmed mean filter with masks of different shapes and sizes, were applied to suppress noise and to smooth pore walls.

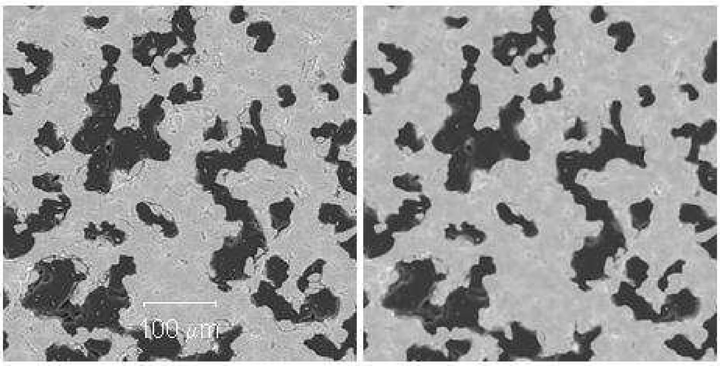

Fig. 1. Raw image of porous material C (left). Solid and void phases are respectively light and dark grey. Spatial filtration of the raw image using an adaptive median filter (right).

Segmentation using a global threshold assigned black or white to each pixel in an image. As a result, binary images (Fig. 2 left), 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. The correctness of our methodology was checked by merging the outline of pores with original image of the appropriate cross-section (Fig. 2, right).

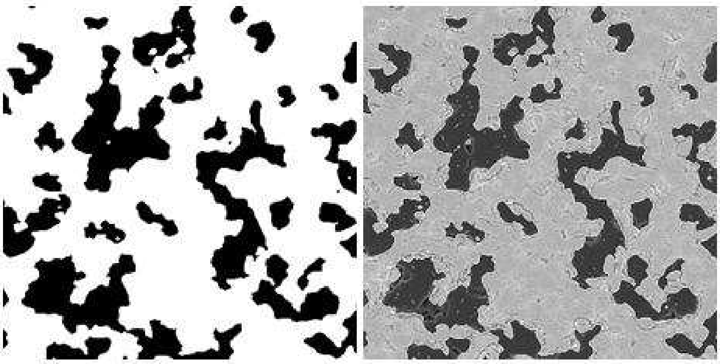

Fig. 2. Segmented (binarized) image. Pores are black. The raw image merged with interface of phases (white curves, right).

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

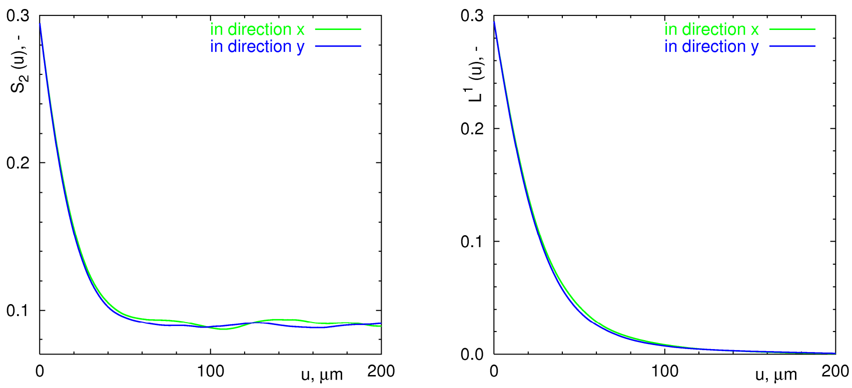

Fig. 3. Macroporous material C. Two-point probability function for the void phase (left), lineal-path function for the void phase (right), both in the principal directions.

area would be close to their counterparts obtained from helium pycnometry, 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 (Fig. 3, left), lineal-path function (Fig. 3, right) and two-point cluster function. These descriptors were used in our modified method of stochastic reconstruction using simulated annealing [3]. An example of obtained replica is shown in Fig. 4.

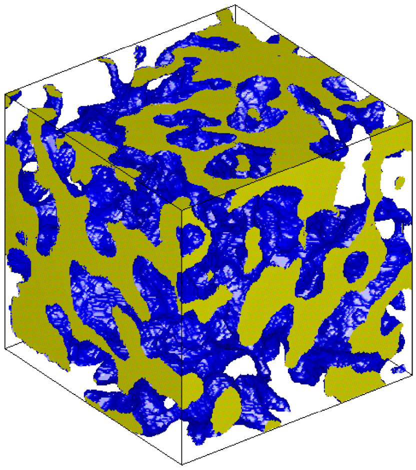

Fig. 4. 3D stochastic replica shown as a subregion of 160×160×160 voxels. Pore orifices are yellow, pore-solid interface is blue, and solid matrix is transparent.

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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