CHARACTERIZATION OF THE PORE STRUCTURE THROUGH MULTISCALE MODEL

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Abstract

Pore-structure directly determines porous material’s macroscopic properties such as permeability or diffusivity. Many related attempts have been conducted experimentally or theoretically, but each method has its limitation.

In this context, a new modeling method has been attempted which takes the pore-structure as three-dimensional pore-network, which, different from other theoretical models, integrates experimental results as the basic input information. Concerning the random nature of pore-structure, a stochastic pore-network has been introduced. Following it, an effective computer generation algorithm has been developed to generate the random pore-scale network. In the new modeling method, the geometries of pores and the corresponding stationary random distribution are defined based on experimental information firstly. The take-and-place method and selection algorithm are employed to realize the pore-network. The effectiveness of this new modeling method has been validated compared with experiment results.

Keywords: Stochastic pore structure, Network modeling, Generation algorithm.

1 INTRODUCTION

Many researchers and engineers have been taking efforts to get insight into pore-structure of porous materials, as the pore geometrical and topological properties directly determines material’s macroscopic properties such as permeability or diffusivity[1].

In this regard, plenty of technical methods, including Mercury intrusion porosimetry (MIP), Scanning electron microscopy (SEM) image analysis, X-ray scattering (SAXS), Nuclear magnetic resonance (NMR), have been employed to measure the microstructure, which give access to the pore-size distribution and the total pore volume. But the above techniques may not identify the connection and location of the pores, and thus building up different pore arrangements with different macroscopic input parameters becomes very important.

Based on the above experimental techniques, the reconstruction of pore structure has been mostly performed by two different models, which are digital images analysis method and MIP
data analysis method. However, when concerning the pore sizes of porous materials range from 1nm to 1mm, 6 orders of magnitude, the above techniques will meet difficulties in generating geometric and physical samples because of the huge workload. Besides, another significant difficulty in using the above pore-network models in a quantitative predictive sense lies in choosing the geometric shape, size, locations, and orientations of the pore bodies and throats so that the amount of detail in the description of the pore space geometry is sufficient to make accurate prediction of macroscopic properties. So a new multi-scale modeling method has been developed which takes the pore-structure as three-dimensional random pore-network, which, different from other theoretical models, integrates experimental results as the basic input information simultaneously. The algorithm takes on the following merits: (1) be suitable to generate random samples with larger length-scale gap due to using $\varepsilon$-size random distribution model. (2) The generated samples have better randomness. It means that the shape, size, locations, and orientations of the pore bodies and throats are completely implemented. (3) be able to generate not only the models with uniform and norm random distribution, but also those with specified distributions obtained from MIP experiment.

2 MULTI-SCALE THEORETICAL MODEL OF THE PORE STRUCTURE

In order to build multi-scale theoretical model of pore structure, we divide porous material into cells. Each cell is a constant $\varepsilon$-cube, Fig.1. As to a cell, we describe pore structure as a spatial network in which larger pores are connected via narrower pores. In the model spheres represent larger pores, while cylinders represent the connections between them. Then we try to establish a computer generation algorithm to generate large numbers of spheres and cylinders.

Random distribution of spheres and cylinders can be characterized as follows: (1) The diameter and location of spheres are random. (2) The diameter and length of cylinders are random, but its location is determined by the location of its connected spheres.

Figure 1 : The set of $\varepsilon$-cube

Thus, the characteristic of random distribution of pores can be represented by the probability density functions of 4 random parameters of spheres and 2 random parameters of cylinders: the shape parameters, namely the diameter of sphere $D_s$, and the location parameters, namely the central points $(x_0, y_0, z_0)$ of the sphere, the diameter of cylinder $D_c$, and the length of cylinder $L_c$. 
3 STOCHASTIC RECONSTRUCTION ALGORITHM

In order to produce a pore-scale network model of porous material that resemble real porous material in the statistical sense, the random sampling principle of Monte Carlo simulation method is used. The model construction process consists of two main parts:

(1) An assembly of randomly distributed spheres, Fig.2. The major factors are the size distribution and spatial distribution of spheres. A bran-new effective generation algorithm called take-and-place method will be considered below. In the take-and-place algorithm[2, 3], the generated spheres are filled into the cubic domain with rejection in such a way that there is no overlapping with spheres already placed. The shape parameters of generated spheres satisfy the specified random distribution model to completely ensure the randomness, and the location parameters can be temporarily considered as a uniform random distribution.

(2) An assembly of randomly distributed cylinders. The major factors are the connection numbers, size and spatial position of the two adjacent spheres.

In order to construct the algorithm suitable to several stochastic parameters, the lemma in [4, 5], namely selection method lemma, is introduced.

3.1 Take-and-place method

Before introducing take-and-place method, it’s necessary to divide the grading pore-size distribution obtained from experiment into segments and calculate volume of spheres and cylinders to be generated within each grading segment. Fig.3.

Take-and-place method contains two processes: take-process and place-process, which are simultaneously performed. It means a sphere generated in take-process is immediately placed into the cube. The two processes are conducted in a sequence starting with the largest size spheres, proceeding until the last sphere of the size range has been placed, and then repeating for successively smaller size spheres.

For the grading segment $[D_i, D_{i+1}]$, the detailed process is as follows:

(1) Calculate the volume of spheres and cylinders to be generated in the grading segment.

(2) Generate a random number defining as the size of a sphere. Assuming that the size $D$ has a uniform distribution between $D_i$ and $D_{i+1}$, it may be taken as $D = D_i + \eta(D_{i+1} - D_i)$ in which $\eta$ is a random number uniformly distributed between 0 and 1. Calculate the volume of each
generated sphere.

(3) Generate random number defining the location of a sphere and place the sphere into the cube. The new sphere will be placed in a reasonable position so that spheres in the cube are not overlapped with previously placed spheres.

(4) Generate cylinders using the method in the next subsection.

(5) Repeat steps 2-4 until the remaining volume of grading segment is less than \( \frac{\pi D_i^3}{6} \), i.e. not enough to generate another sphere. Then it will be calculated into next grading segment.

(6) Repeat all above steps for next grading segment and then again for successively smaller size grading segments, until the last sphere of the smallest size has been generated and placed.

Figure 3: Random selected of sphere sizes in a Mercury injection experiment

3.2 Cylinders generation method

As for generation method of cylinders, connection number is a vital concept, which denotes the number of cylinders connected to a sphere. And it reflects the connectivity of the whole spatial pore-network. Diameter of cylinder satisfies a specific distribution, but the length of cylinder is obtained from the distance of two adjacent spheres. Since the layout of cylinders is entirely dependent on the distribution of the sphere, it needs not be separately considered. The detailed process is as follows:

(1) Generate a random integer number defining as the connection number of each generated sphere, then record them as \( c_n \).

(2) For a sphere, search all of its adjacent spheres whose distance is lower than a given number.

(3) If connection number of both is bigger than zero, generate a cylinder between them and \( c_n = c_n - 1 \). It is proposed that the diameter \( D_c \) of cylinder be taken as \( \mu \) times the smaller value of \( D_a \) and \( D_b \), where \( \mu \) is a random number uniformly distributed between 0 and 1. The length of cylinder is the distance of two adjacent spheres.

(4) Repeat all above steps for next sphere, until all cylinders of the last sphere has been generated.

4 EXAMPLE

For validation of this new modeling method, a theoretical pore-network based on the result of mercury intrusion porosimetry (MIP) was constructed.
At first a unit cell with the volume of 1.0E-6 is set to reconstruct the pore-network. And the central points \((x_0, y_0, z_0)\) of spheres obey the uniform distribution in \([0, 0.01] \times [0, 0.01] \times [0, 0.01]\). Then porosity of the sample was measured and found to be with MIP test as 0.03. In addition, a series of representative diameters were selected from the experimental cumulative pore volume curve. The principle to choose the diameter is to let their differential volume as the same. In this simulation, totally ten diameters were selected, which is plotted in Fig.4. Moreover, the chamber-diameter distribution is obtained from the experimental mercury intrusion curve, while the throat diameter distribution estimated. Finally, the mean and maximum coordination number is set as 4 and 20.

From fig.4, it illustrates Mercury intrusion in the theoretical pore-network is simulated and compared with the corresponding one of the experimental curves. And fig.5 plots the TSD by differentiating the mercury intrusion curve. The simulated pore size distribution is very close to the corresponding ones of the sample, which indicates the simultaneous estimation of the network parameters is possible by this new modeling method.

![Image](image1.png)

**Figure 4:** Cumulative pore volume at different pore diameter: Mercury intrusion in the theoretical pore-network compared with the experimental curves

![Image](image2.png)

**Figure 5:** Illustration on TSD: Mercury intrusion in the theoretical pore-network compared with the experimental curves

**5 CONCLUSIONS**

An effective computer generation algorithm for porous materials to generate a random pore-network model is proposed in this paper. The model construction process consists of two
main parts: the assemblies of randomly distributed spheres and cylinders. The spheres are
generated according to a given grading size distribution curve which obtained from an
experiment. The generation algorithm of the location parameters incorporates a take-and-
place method and a selection algorithm. Especially, for the selection algorithm, it can not only
simulate the model with a uniformly random distribution, but also simulate those with a
special random distribution. And it can also be extended to simulate the mixed model of
several different random distributions.

In accordance with the connection number of each sphere, the cylinders are generated with
diameter being the random number between 0 and the diameter of smaller sphere. Length of
cylinders can be determined by the distance of two adjacent spheres. Connection number is
used for study because it’s a key step to provide a pore-network with good connectivity.

In the future our research will focus on using the pore-network to predict flow properties,
such as relative permeability and capillary pressure, which can verify the significance of
computer generation algorithm.

6 REFERENCES

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