Multiscale geometrical reconstruction of porous structures

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Multiscale percolation systems (MPSs) were proposed to study invasion processes in porous media with a large pore size distribution, considering the porous section as a polydisperse structure that modifies its geometrical structure when the scale of observation is changed. Multiscale models are nonregular percolation systems and do not have the following limitations common to classical percolation systems: (i) It is not necessary to choose a particular value for the coordination number Z nor to establish a particular distribution law for it and (ii) constrictions appears naturally as pores of smaller diameters connecting pores of greater diameters, as the result of superposing different scales. A fundamental question that arises in this method is related to the conservation of the spatial connectivity between the pores, which is very important if MPS models are to be used for simulating fluid retention and transfer. The present work is focused on this problem. It is shown that, although conserving the classical correlation function at the object level, i.e., pores, the use of a MPS as a representation of a porous medium does not allow for the conservation of the geometrical structure of clusters of connected pores. An improved MPS model is discussed. [S1063-651X(96)08407-3]

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I. INTRODUCTION

Microscopic models for simulating fluid retention and transfer in porous media are frequently monodisperse models based on random percolation networks of sites and/or bonds interacting between themselves in a single scale. Classically, sites are randomly distributed in a network with a constant or variable coordination number Z, which is the number of sites that are neighbors of each site in the network. The diameter of the bond connecting two contiguous sites is randomly chosen so as to remain smaller than the diameters of the connected sites. Several well-known problems are associated with this construction procedure: (i) It is very difficult to choose a particular constant coordination number Z for the porous structure or to ascertain a realistic distribution law for this parameter, (ii) it is very difficult to access the size distribution of constrictions, and (iii) for simplicity reasons, networks are frequently spatially noncorrelated.

Mercury intrusion and sorption isotherms results have been used to estimate the size distribution of constrictions [1,2]. In general, several parameter models are needed in this kind of work, which are adjusted to fit the model to experimental data. In fact, the introduction of bonds in the percolation system is frequently a necessary hypothesis in percolation models due to the lack of information about the spatial distribution of pores. Chatzis and Dullien [1] and Daïan and Saliba [2] used a local correlation between throat size and pore size given by a relationship between the cumulative distributions of throats and pores. Mayagoitia *et al.* [3] have also considered a local correlation between a site and the contiguous bond, generated by the conditional probability related to the impossibility of connecting a site with a bond greater in size. Spatially correlated networks of sites and bonds were considered, e.g., by Renault [4] to study the influence of spatial correlation on the percolation threshold and by Ioannidis and Chatzis [5,6] and Tsakiroglou and Payatakes [7] to study the effect of spacial correlation on mercury intrusion.

Recently, image analysis methods used over pictures of highly polished surfaces of porous materials, taken with an electron scanning microscope, have been used to describe the porous structure [8–12]. Aperture and median line graphics methods [10,13] enable the statistical investigation of porous sections, including the statistical description of constrictions and connectivity between pores. By assuming isotropy, three-dimensional percolation networks can thus be constructed from two-dimensional (2D) porous sections, conserving the size distribution of pores and constrictions and the distribution law for the coordination number [10].

A multiscale approach is used in the present article. The porous section is conceived as a polydisperse structure that modifies its geometrical structure when the scale of observation is changed. This conception is in accordance with the fractal (in the sense of *broken*, as in Mandelbrot [14]) nature of porous materials: geometrical parameters such as porous volume V and porous surface S require the use of a measuring scale l and increase their values as l decreases. Without taking the technical difficulties into account, such as attainable resolution when using electron scanning microscopy or any other kind of measuring method, this description appears to be specially suitable for the geometrical description of porous media with a large pore size distribution. Another difficulty comes from the limitations of the geometrical models, necessary for simplicity in the geometrical description.

Multiscale models were introduced by Neimark [15], called multiscale percolation systems (MPSs). At the first scale, a mosaic of blocks of size r_1 is constructed. These blocks are classified as pores (X blocks), solid matter (Y blocks), and blocks of pores with sizes smaller than r_1 (Z blocks), which are *randomly* distributed in accordance with a previously known pore size distribution. In a second scale $r_2 = r_1/n_1$, where n_1 is an integer, each block Z is farther

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segmented in blocks X, Y, and Z of size r_2 and so on. At each scale i the construction process of the MPS preserves the volume fraction of pores with size equal to or greater than r_i, v_i^X, and the volume fraction of solid matter v_i^Y observed at this scale. The remaining volume fraction $v_i^Z = 1-(v_i^X + v_i^Y)$ is considered to be composed by porous matter, made by pores with diameters smaller than r_i and not observed at scale i.

Based on Neimark's model, Daïan [16] proposed a simplified version of the method, randomly distributing the pores at each scale, starting from the smaller diameters and multiplying the scale length by 2 at each step. At each scale, pores are randomly distributed in accordance with their volume fraction obtained from the pore size distribution. In this method, no Z blocks are introduced in the structure, in order to reduce the number of volume fractions to be identified. Reconstruction of the medium is performed by superposing the different scales. See also Daïan, Xu, and Quenard [17].

Multiscale models as conceived by Neimark and Daïan are nonregular percolation systems and do not have the first two limitations mentioned in the first paragraph of the present section. In fact, (i) it is not necessary to choose a particular value for the coordination number Z nor to establish a particular distribution law for it and (ii) constrictions appear naturally as *pores* of smaller diameters connecting pores of greater diameters, as the result of superposing different scales.

Another important question that arises in this method is related to the third limitation mentioned in the first paragraph of the present section, i.e., the conservation of the spatial correlation of the pores when the different scales are superposed: although the pores are not spatially correlated at a given scale, the correlation function will be different from zero for displacements smaller than the greater pore diameter found in the microstructure, when calculated over the reconstructed section. The question to be posed is *whether the reconstruction method preserves the correlation function measured over the original 2D binary representation of the porous section*. The present work is focused on this problem.

II. STATISTICAL PARAMETERS OF 2D POROUS SECTIONS

Let S be a section of a porous medium, given by a 2D binary representation like the one shown in Fig. 1, where the porous phase is represented in black and the solid matrix in white [18]. It is supposed that the porous medium is isotropic and that S is large enough to enable statistical homogeneity. Two binary representations related to any two different sections of the medium will be thus statistically equivalent. In the same way, S will display all the statistical information at this representation.

Classically, a phase function Z is defined as

$$Z(\mathbf{x}) = \begin{cases} 1 & \text{when } \mathbf{x} \text{ belongs to the pore space} \\ 0 & \text{otherwise,} \end{cases} \tag{1}$$

where $\mathbf{x}$ denotes the vector giving the position in the plane of S. In fact, $\mathbf{x}$ denotes the set of 2-uples (x_1, x_2), where x_1, x_2 are integers, multiples of the measuring unit, i.e., the pixel. The apparent porosity, i.e., the void fraction *at the selected scale*, can be obtained as

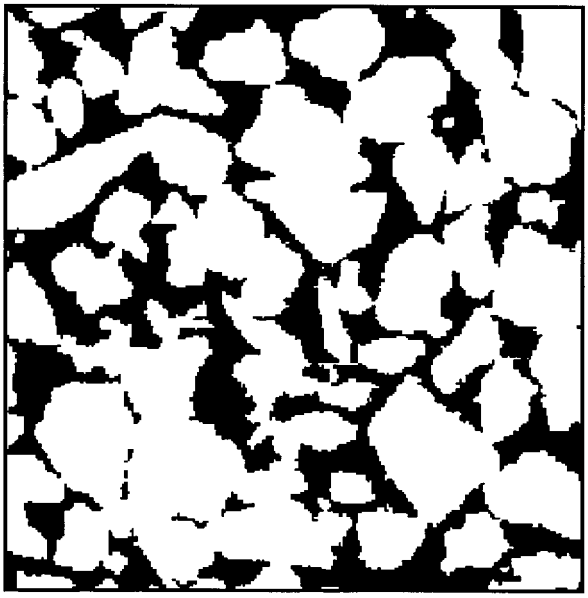

FIG. 1. Binary image of a polished section of Fontainebleau sand (Fontainebleau, France): pores are shown in black and the solid matrix in white.

$$\varepsilon = \langle Z(\mathbf{x}) \rangle, \tag{2}$$

where $\langle\ \rangle$ means statistical average in the sample space. A correlation function can also be written as

$$C(\mathbf{u}) = \langle Z(\mathbf{x}) Z(\mathbf{x}+\mathbf{u}) \rangle \tag{3}$$

for each arbitrarily chosen $\mathbf{u}$, where $\mathbf{u}$ is a displacement in the plane of the porous section. Assuming an isotropic porous distribution, the correlation function will only depend on $u = |\mathbf{u}|$ and can be written as

$$C(u) = \langle [Z(x_1, x_2)][Z(x_1+u, x_2)] \rangle. \tag{4}$$

The correlation function decreases from $C(u) = \varepsilon$ for $u = 0$ to $C(u) = \varepsilon^2$ for large values of u. Similarly, the normalized covariance function can be defined as

$$R(u) = \frac{\langle [Z(x_1, x_2) - \varepsilon][Z(x_1+u, x_2) - \varepsilon] \rangle}{\langle [Z(x_1, x_2) - \varepsilon]^2 \rangle}, \tag{5}$$

with values between 1 (for $u = 0$) to 0 (for large u).

As implied by Eq. (3), the correlation function can be obtained by displacing the binary representation over itself in the x_1 direction (or x_2), using multiples of the cell dimensions and measuring the void fraction related to the intersection, i.e., the frequency of outcomes corresponding to two superposed black cells. This method is described in more details by Adler [19] and Philippi *et al.* [9].

A. Connectivity function

The correlation function is related to the spatial correlation between two arbitrarily located pixels belonging to the porous phase (black phase) when separated by u and is not to

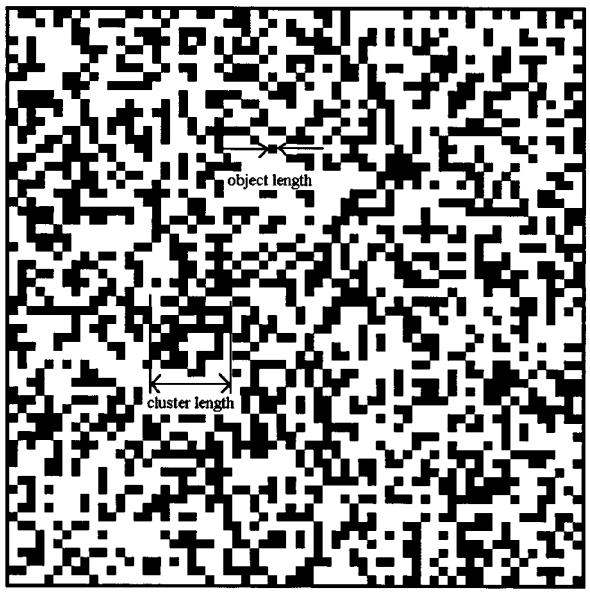

FIG. 2. Artificially generated porous section: the black phase is composed by identical black square objects with linear dimension l_0 *randomly* distributed in a square section with a number fraction $p<p_c$. The cluster length l_c is identified in the figure, considered to be the linear length of the greatest cluster of connected black objects present in the section.

be confused with the probability of finding two black pixels separated by u, *but belonging to the same connected cluster*. In fact, this second probability would be, in principle, more appropriate to describe the connectivity between any two black pixels when separated by u and will be defined by the introduction of a new phase function

$$P(\mathbf{x})=\begin{cases} k & \text{when } \mathbf{x} \text{ belongs to the porous phase } k \\ 0 & \text{otherwise.} \end{cases} \tag{6}$$

A *connectivity function* $\zeta(\mathbf{u})$ can thus be defined as

$$\zeta(\mathbf{u})=\langle \delta(P(\mathbf{x}),P(\mathbf{x}+\mathbf{u}))\rangle, \tag{7}$$

where $\delta(i,j)$ is 1 if $i=j\neq 0$ and 0 otherwise. The phase function $P(\mathbf{x})$ can be obtained by labeling the connected black clusters present in the porous section S. In the present work, this was performed by using the labeling algorithm developed by Hoshen and Kopelman [20].

The connectivity function $\zeta(\mathbf{u})$, defined as above, shows a very interesting behavior when used to describe isotropic porous sections S. Some tests were performed with an artificially generated porous section, when the black phase is composed by the union of identical black square objects *randomly* distributed in a square section with a linear dimension l, great enough to ensure statistical homogeneity (Fig. 2). Taking p as the number fraction of black objects, the results indicate that, whereas the classical correlation function has the *same behavior* every time, decreasing from ε (at $u=0$) to ε^2, at $u\sim l_0$, where l_0 is the length of the identical black objects distributed in the black phase, (i) for $p<p_c$, where p_c corresponds to the percolation threshold in two dimensions, $\zeta(u)$ decreases from ε (at $u=0$) to 0 (at $u\sim l_c$ the

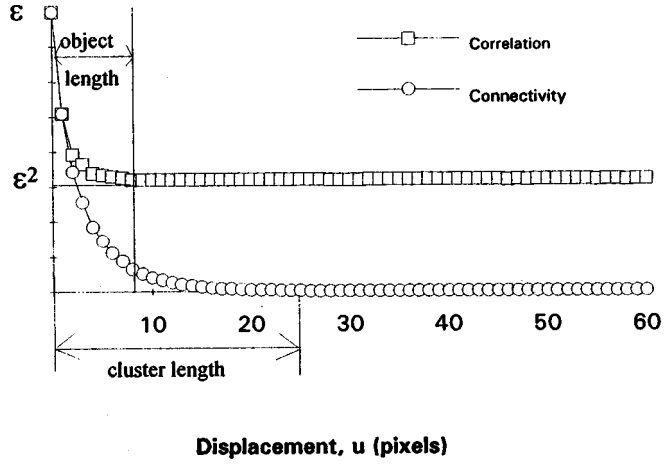

FIG. 3. Comparison between the classical correlation function $C(u)$ and the connectivity function $\zeta(u)$, presently defined, for an artificially generated porous section with identical black objects, with linear length l_0, randomly distributed in the section. The number fraction of black objects p is smaller than p_c. $\zeta(u)=0$ only for $u>l_c$, where l_c is the cluster length, whereas $C(u)=\varepsilon^2$ for $u>l_0$.

cluster length, defined in this work as the length of the greatest cluster present in the porous section), which is a very interesting property, since the cluster length l_c increases with the proportion p of black objects and indicates that $\zeta(u)$ *is modified by the fashion the objects are grouped to form clusters* (Fig. 3); and (ii) for $p>p_c$, $\zeta(u)$ decreases from ε (at $u=0$) to ε_c^2, where ε_c is the *connected* porosity of the porous section, i.e., the volume fraction of pores that are connected to the outer surfaces (Fig. 4).

Note that the definition of the connectivity function is necessary for the analysis of 2D sections of a 3D porous medium: two clusters that are not connected in two dimensions may be connected between themselves in the third dimension. However, two different 2D sections of a given 3D porous medium must present the *same* connectivity function, if the medium can be supposed isotropic.

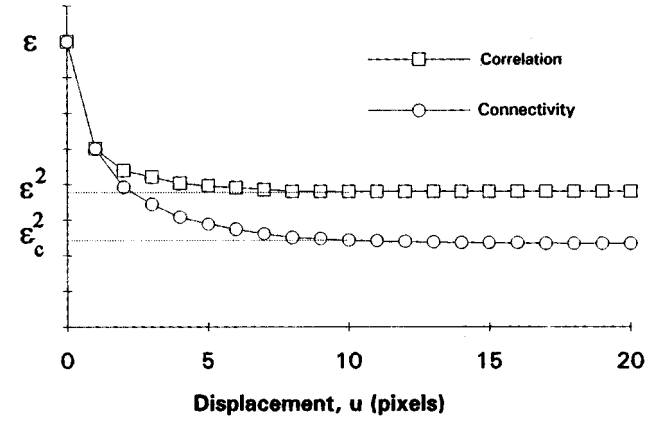

FIG. 4. Comparison between the classical correlation function $C(u)$ and the connectivity function $\zeta(u)$, presently defined, for an artificially generated porous section with identical black objects, with linear length l_0, randomly distributed in the section. The number fraction of black objects p is greater than p_c. $\zeta(u)=\varepsilon_c^2$ for larger values of u, whereas $C(u)$ has the same behavior presented in Fig. 3, reducing to ε^2 for $u>l_0$.

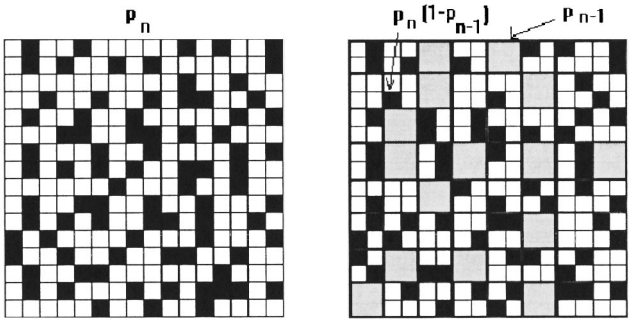

FIG. 5. Superposition of scales n and $n-1$.

Reconstruction of S means generation of 2D or 3D sections preserving the moments of the phase function $Z(\mathbf{x})$, including the apparent porosity ε and all its higher-order moments. In the present paper, the use of multiscale percolation systems for the reconstruction of porous media is discussed. It is demonstrated that the method allows one to preserve the apparent porosity ε and the classical correlation function $C(u)$. However, it is also shown that the connectivity function $\zeta(\mathbf{u})$ is not preserved due to the random spatial distribution of pores, at each scale, in a MPS. An improved MPS reconstruction method is briefly discussed.

III. MULTISCALE 2D OR 3D RECONSTRUCTION FROM 2D SECTIONS

Following Neimark [15] and Daïan, Xu, and Quenard [16,17], pore sections will be supposed to be a superposition of square (2D) or simple cubic (3D) networks. Pores will be supposed to be squares (2D reconstruction) or cubes (3D reconstruction) of linear size D_i. The class $i=1$ corresponds to the larger diameters and the class $i=n$ to the smaller ones. For each class i, $D_i=2D_{i+1}$:

$$D_1=2D_2=4D_3=\cdots=2^{n-1}D_n, \tag{8}$$

which is equivalent to taking the lowest integer 2 as a constant scale factor [16,17]. The scale n corresponds to a *one-sized* distribution of L_n^d pores with diameter D_n and cells of solid matter with diameter D_n (or cells of porous matter, with pore diameters smaller than D_n). The symbol d means the dimension of the MPS: $d=2$ in 2D and $d=3$ in 3D MPS. The scale $n-1$ corresponds to a two-sized distribution of pores of diameters D_n and pores of diameter D_{n-1}. At this scale the number of cells in the MPS is L_{n-1}^d, where $L_{n-1}=L_n/2$. Let v_n be the volume fraction of class n, apparent at scale 1. Let p_n be the fraction of pores of class n, which will be distributed *at random* at scale n. Superposition of pores of class $n-1$ with pores of class n, at the scale $n-1$, will mask part of the volume fraction of pores from class n, at this scale (Fig. 5) and only a $p_n(1-p_{n-1})$ fraction of pores of class n will be apparent at scale $n-1$. In fact, both classes of pores were distributed at random and independently at each correspondent scale. At scale $n-2$ there will be $p_n(1-p_{n-1})(1-p_{n-2})$ pores from class n and $p_{n-1}(1-p_{n-2})$ pores from class $n-1$. Following recursively, after $n-1$ superpositions, the apparent volumes v_i, $i=1,2,\ldots,n$, can be written as

$$\begin{aligned} v_n&=p_n(1-p_{n-1})\cdots(1-p_1),\\ v_{n-1}&=p_{n-1}(1-p_{n-2})\cdots(1-p_1),\\ &\cdots,\\ v_1&=p_1, \end{aligned} \tag{9}$$

which constitute a set of n equations that can be solved for the unknowns $p_1,p_2,\ldots,p_n$. Let V_i be the total porous volume, apparent at scale i,

$$V_i=\sum_{j=1}^{i} v_j. \tag{10}$$

Let ε_i be the apparent porosity of the multiscale system, considered as the superposition of scales n to $i+1$. The total porosity ε may thus be written as

$$\varepsilon=V_i+(1-V_i)\varepsilon_i \tag{11}$$

and, consequently,

$$\varepsilon_i=\frac{\varepsilon-V_i}{(1-V_i)}. \tag{12}$$

At each i scale, the correlation function will positive for displacements smaller than D_i. In fact, although the pores i are distributed at random at each scale i, the superposition of pores of class $i-1$ on the i scale will make correlated the pores at displacement level i. This is the basic principle of the present reconstruction method. Two classes of problems may be thus established: (i) to calculate the correlation function for displacements u_i smaller than D_1 as a function of the volume fractions v_i apparent at scale 1 (direct problem) and (ii) to calculate the volume fractions v_i apparent at scale 1 from the measured values of the correlation function (inverse problem). In the following, the two problems are formulated for a given porous section, associated with a single binary representation.

A. Direct problem

The MPS is considered to be infinite in size. Let C_1 be the correlation value related to a D_1 displacement, i.e., the intersection volume between the pores of the original MPS and the pores of this same system displaced by D_1. As pores of class 1 are considered as the greater geometrical entities present in the multiscale system, a D_1 displacement of the MPS will put each class of pores in intersection with anyone of the pores present in the MPS, with a proportion ε. The probability of intersection will thus be

$$C_1=v_1\varepsilon+v_2\varepsilon+v_3\varepsilon+\cdots=\varepsilon^2. \tag{13}$$

Consider now a $D_2=D_1/2$ displacement and let C_2 be the associated correlation (Fig. 6). In this case, one-half of the pore of class 1 will intercept itself and the other half will intercept any one of the pores of the MPS with a probability of intersection $v_1/2+(v_1/2)\varepsilon$. For pores of class 2, half of these pores, labeled with a circle in Fig. 6, will surely not intercept pores of class 1 for a D_2 displacement and the other half may intercept with any one of the pores in the MPS. The probability of intersection associated with the pores of class 2 when submitted to such a displacement will thus be

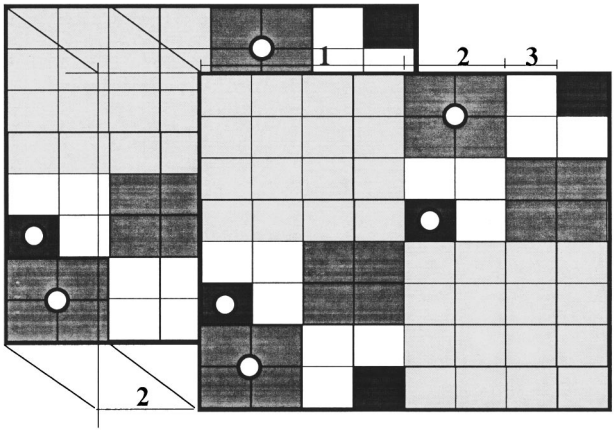

FIG. 6. Calculation of the correlation C_2 by displacing the MPS by D_2. Pores of classes 2 and 3 labeled with a ○ cannot intercept pores of class 1, with a D_2 displacement.

$(v_2/2)\varepsilon_1+(v_2/2)\varepsilon$, where the first term of this sum is the conditional probability that half of the pores of class 2 intercept another pore, given that they will never intercept pores of class 1 with a D_2 displacement. Applying the same reasoning for pores of class 3, 4,..., the following expression will be obtained for C_2:

$$C_2=\left(\frac{v_1}{2}+\frac{v_1}{2}\,\varepsilon\right)+\left(\frac{v_2}{2}\,\varepsilon_1+\frac{v_2}{2}\,\varepsilon\right)+\left(\frac{v_3}{2}\,\varepsilon_1+\frac{v_3}{2}\,\varepsilon\right)+\cdots$$
$$=\frac{\varepsilon^2}{2}+\frac{(\varepsilon-V_1)}{2}\,\varepsilon_1+\frac{v_1}{2}. \tag{14}$$

Proceeding with the same reasoning for C_3,

$$C_3=\left(\frac{3v_1}{4}+\frac{v_1}{4}\,\varepsilon\right)+\left(\frac{2v_2}{4}+\frac{2v_2}{4}\,\varepsilon_1+\frac{v_2}{4}\,\varepsilon\right)$$
$$+\left(\frac{2v_3}{4}\,\varepsilon_2+\frac{v_3}{4}\,\varepsilon_1+\frac{v_3}{4}\,\varepsilon\right)+\cdots$$
$$=\frac{\varepsilon^2}{4}+\frac{3v_1}{4}+\frac{2v_2}{4}+(\varepsilon-V_1)\,\frac{\varepsilon_1}{4}+(\varepsilon-V_2)\,\frac{2\varepsilon_2}{4}. \tag{15}$$

For an arbitrary D_j displacement, the associated correlation will be

$$C_j=\frac{\varepsilon^2}{2^{j-1}}+\sum_{i=1}^{j-1}\frac{(\varepsilon-V_i)\varepsilon_i}{2^{j-i}}+\sum_{i=1}^{j-1}\frac{2^{j-i}-1}{2^{j-i}}\,v_i, \tag{16}$$

which enables the calculation of C_j from given values of the pore sizes distribution $v_1,v_2,\ldots,v_N$.

B. Inverse problem

From Eq. (16), the volume V_j can be explicitly related to the correlation values by

$$V_j=\frac{C_j-2C_{j+1}+\varepsilon^2}{C_j-2C_{j+1}+2\varepsilon-1}, \tag{17}$$

which means that v_j is uniquely determined from the correlations calculated at the displacements D_j, using

$$V_n=\varepsilon,\quad v_j=V_j-V_{j-1}. \tag{18}$$

Equations (16) and (17) imply that (i) for a given pore size distribution there is one and only one associated correlation function that conserves the apparent porosity ε and, conversely, (ii) for a given correlation function there is one and only one pore size distribution for the given apparent porosity ε. In other words, in the present conception, there is a one-to-one correspondence between the pore size distribution and the correlation function, i.e., the MPS model has *one and only one* correlation function. This one-to-one correspondence ensures that the correlation function measured at the MPS or calculated with Eq. (16) will be the same as the correlation function measured at the original 2D binary section of the porous section, *when this section can be represented by a MPS.*

IV. VALIDATION OF THE MODEL

Equation (16) was validated against measured values of the correlation for four artificially Monte Carlo generated 2D multiscale systems of size 8192×4096 pixels. Correlation values were measured using the method described by Adler [19] and by Philippi *et al.* [9], assuming isotropy, and calculated using the theoretical expression Eq. (16). Table I shows the results. The first column gives the theoretical values of v_i used for Monte Carlo generation of the MPS. The second column gives the values of v_i measured at the MPS after Monte Carlo generation, graphically computing the number of cells of each class. These values where used for calculating the correlations. Column 3 presents the error between the theoretical value of the correlations [given by Eq. (16)] and their corresponding measured values over the MPS. It is seen that (i) errors are very small, remaining smaller than 0.250% for all displacements, and (ii) errors increase with increasing displacements.

V. MULTISCALE RECONSTRUCTION OF THE POROUS STRUCTURE OF A CEMENT AND LIME PASTE

Figure 7 shows a binary representation of a 3200× magnification picture of a cement and lime paste, taken with a scanning electron microscope (see [9] for details). Each pixel corresponds to a 625×625 Å^2 square. Pores of diameters smaller than 625 Å are thus not apparent at this magnification. The apparent porosity at this magnification was calculated as 0.4714.

Volume fractions were determined for each pore diameter using the aperture method from image analysis [13]. The d_{3-4} metric was used for the determination. Figure 8 shows two balls, in this metric, corresponding to the most elementary structural elements that can be used in aperture operations, with diameters of 2 and 4 pixels (associated with 1250 and 2500 Å), respectively. The smallest pore diameter that can be found using this metric is thus 1250 Å. The cumulative volume fractions corresponding to 1250, 2500, 5000, 10 000, and 20 000 Å were used to construct the MPS model shown in Fig. 9, using Eq. (9) to take the effect of superposition into account. Several MPSs were generated and the

TABLE I. Comparison between measured and calculated values of the correlation function for four artificially Monte Carlo generated, 2D porous sections of size 8192×4096 pixels.

v_i (theoretical values)	v_i (measured values)	Displacement	Errors between measured and calculated values of C_i (%) $10^2\left\|\frac{C_i^{\text{meas}}-C_i^{\text{theor}}}{C_i^{\text{meas}}}\right\|$
$v_1=0.1$	$v_1=0.099$	D_1	0.224
$v_2=0.1$	$v_2=0.100$	D_2	0.111
$v_3=0.1$	$v_3=0.100$	D_3	0.092
$v_4=0.1$	$v_4=0.100$	D_4	0.050
$v_5=0.1$	$v_5=0.100$	D_5	0.016
$v_1=0.1$	$v_1=0.099$	D_1	0.194
$v_2=0.1$	$v_2=0.100$	D_2	0.098
$v_3=0.2$	$v_3=0.200$	D_3	0.044
$v_4=0.2$	$v_4=0.200$	D_4	0.021
$v_5=0.3$	$v_5=0.300$	D_5	0.011
$v_1=0.1$	$v_1=0.099$	D_1	0.201
$v_2=0.2$	$v_2=0.201$	D_2	0.103
$v_3=0.3$	$v_3=0.300$	D_3	0.052
$v_4=0.2$	$v_4=0.200$	D_4	0.022
$v_5=0.1$	$v_5=0.100$	D_5	0.011
$v_1=0.3$	$v_1=0.299$	D_1	0.200
$v_2=0.2$	$v_2=0.201$	D_2	0.100
$v_3=0.2$	$v_3=0.200$	D_3	0.046
$v_4=0.1$	$v_4=0.100$	D_4	0.029
$v_5=0.1$	$v_5=0.100$	D_5	0.013

correlation function was measured over the MPSs and calculated using Eq. (16). Table II shows the results for three MPSs with size 4096×4096 pixels constructed using different random generators. A comparison is also performed with respect to the values of the correlation function measured over the original porous section (Fig. 7). The agreement is quite good, showing that MPS reconstruction does not modify the spatial correlation of the porous structure *at the object level*.

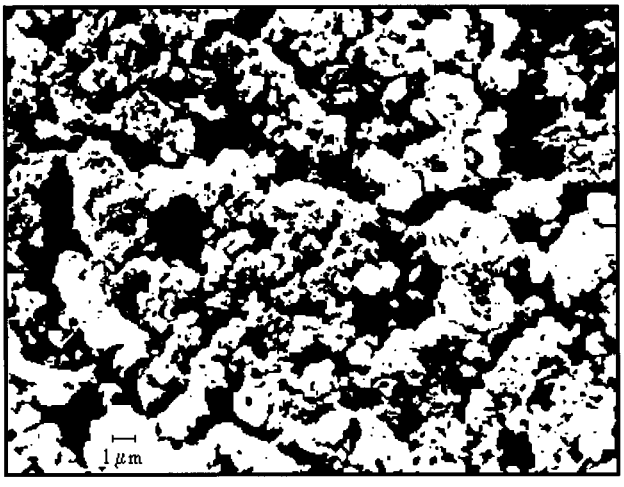

FIG. 7. Binary representation of a 3200× magnification picture of a cement and lime paste [9].

VI. MPS RECONSTRUCTION AND CONNECTIVITY FUNCTION

Visual inspection of Figs. 7 and 9 indicates that the spatial correlation between pores, forming clusters of connected objects in two dimensions, was not conserved in MPS reconstruction. In fact, as already mentioned, the main limitation of MPS models is related to the randomness hypothesis at each scale. In the present section, the connectivity function defined in Sec. II A is used to quantify this limitation, by measuring $\zeta(u_i)$ on the original porous section (Fig. 7) and at the MPS model shown in Fig. 9. Results are shown in Fig.

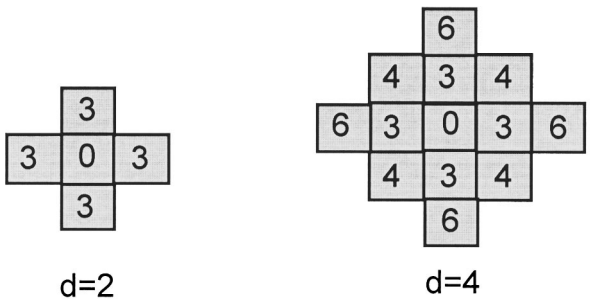

FIG. 8. Balls, in metric d_{3-4}, with diameters of 2 and 4 pixels, respectively.

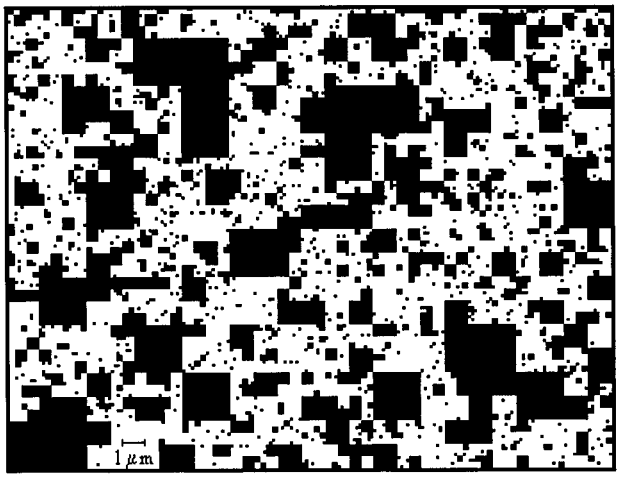

FIG. 9. MPS reconstitution of the porous section shown in Fig. 7.

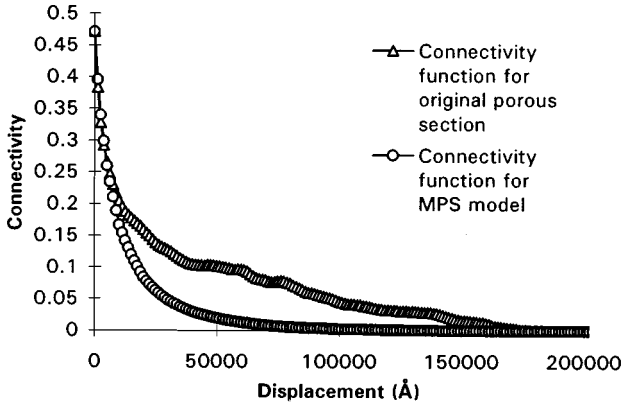

FIG. 10. Comparison between the measured values of the connectivity function at the original porous section and at the MPS model.

10. It can be noticed, first of all, that both functions converge toward zero, related to the case, previously mentioned, where the apparent connected porosity of the section is zero, while the real medium is probably connected in three dimensions. Figure 10 shows a great discrepancy between the measured values of the connectivity function. The shape of the curves are sensibly different and the correlation length of the MPS is about two times smaller than in the original image. Although conserving, in the case of the medium presently studied, the correlation function at the object level, i.e., pores, MPS reconstruction, as performed here, is not able to conserve the geometrical structure of *clusters* of connected pores. This is an important limitation when the method is used to reconstitute 3D porous media for simulating equilibrium and transfer processes, which are conditioned by the topology of the porous structure, e.g., drainage and fluid transfer.

Another limitation of MPS models is related to the first one, discussed above, although intrinsically more complicated to solve. In fact, in the MPS construction method, pores are considered as objects with the same linear dimension in orthogonal directions: squares or cubes. Porous sections having pores with large length (l) to width (w) ratios (e.g., cracks) cannot be represented by MPS models as conceived in the present paper. In fact, pores with large aspect ratios l/w are considered here as a set of squares (or cubes) with length l equal to the width w of the pore (Fig. 11). In the MPS construction process, these squares (or cubes) are distributed at random at the scale that corresponds to w, eliminating the connectivity of the original porous section. Cracks can be viewed as *clusters of connected pores* and, in this case, the failure of MPS models to represent cracked porous sections can be reduced to the first limitation above discussed, reducing the problem to finding a MPS model, suitable to conserve the connectivity function discussed in Sec. II A. This does not appear to be possible by using the randomness hypothesis at each scale.

VII. DISCUSSION

In the present work a MPS reconstruction method is discussed, when applied to isotropic porous sections. The connectivity function is defined. This function is the probability of finding any two pixels belonging to the same phase, *in the same cluster of connected pixels*, when separated by a given displacement u. Results show that, although conserving the classical correlation function for porous sections that are able to be represented by MPS models, MPS reconstruction, as performed here, fails to conserve the connectivity function.

A more general reconstruction method based on MPS has been proposed [17,21,22] in order to describe the pore space accessible to fluids, i.e., the pore space connected at a large scale. The porous phase is not represented by the MPS itself, but by the multiscale 3D infinite cluster of the MPS. In this type of reconstruction, the volume fraction of each class in the total MPS is calculated, using renormalization functions, from the corresponding volume fraction present in the infinite cluster and taken as the measured values v_i, given by Eq. (9), on the original porous section. The elements of each

TABLE II. Correlation values for three MPSs of size 4096×4096 pixels using different random generators.

Displacement (Å)	Actual values	Calculated at MPS 1	Calculated at MPS 2	Calculated at MPS 3	Measured at MPS 1	Measured at MPS 2	Measured at MPS 3
1250	0.3955	0.3971	0.3967	0.3981	0.3973	0.3960	0.3962
2500	0.3408	0.3462	0.3456	0.3470	0.3463	0.3448	0.3451
5000	0.2890	0.2840	0.2838	0.2849	0.2842	0.2827	0.2830
10000	0.2462	0.2380	0.2379	0.2390	0.2384	0.2370	0.2373
20000	0.2383	0.2219	0.2226	0.2230	0.2227	0.2216	0.2218

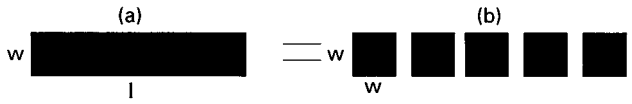

FIG. 11. MPS reconstitution (b) of an object (a) with large length (l) to width (w) ratios.

class belonging to the infinite cluster are thus not randomly distributed in the space as in the total MPS and therefore a certain correlation is introduced in the descriptive structure. In fact, one can expect that using such a method would allow one to improve the results from the point of view of the connectivity function of the reconstructed section. Unfortunately, the identification of the representative volumes to be randomly distributed at each scale, starting from the measured values of the connectivity function is presently not possible, because no equation comparable to Eq. (17) exists for the connectivity function. An analysis concerning the preservation of the connectivity function in 2D sections of the 3D MPS generated by using such a method is presently being undertaken and is planned to be the subject of another paper.

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