The reachable volume fraction in porous media in the vicinity of percolation threshold: a numerical approach used on multi-scale Boolean schemes

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***Abstract*—New morphological descriptors of complex porous networks are introduced and validated in this paper. These descriptors are based on the concept of "reachable volume fraction" here applied on multi-scale Boolean schemes; this fraction is computable for percolating spheres using step by step erosions of the porous network, providing information about the percolation strength of spherical particles with increasing radius. This process yields a critical radius, which, together with the dynamic reachable volume fraction provide a characterization of the porous media.**

Keywords*—Porous networks, Mathematical morphology, Percolation-threshold, Boolean schemes, Multi-scale, Geodesic distance transform, Reachable volume fraction

I. Introduction

Critical percolation-threshold is a crucial morphological descriptor for porous media in filtration systems and diphasic materials in conductive devices [1], [2]. Several approaches can be used to estimate this characteristic: probability formalism [3], [4], topology [5] or excluded volume [6], [2] for instance. It can be defined as a critical volume fraction [7] for an infinite volume size [8].

We propose a complementary approach of the critical percolation-threshold study, leading to new descriptors based on the reachable volume fraction as a function of the radius of a penetrating sphere. In this way, porous media may be characterized by such a discrete curve or its critical point (last one), that we will name descriptors in the sequel.

Firstly, we recall the link between these new descriptors and the critical percolation-threshold. Then we focus on the numerical study of single-scale Boolean schemes [9], [1], [10], for which we have a reference value, with a potential speed up of critical percolation-threshold computation. Finally we apply our new characterization to complex multi-scale Boolean schemes of platelets.

II. Method

Critical radius

For a Boolean scheme A, according to [11], the density θ of objects A' is given by:

$$1 - V_v = \exp(-\theta.\bar{V}(A')) \tag{1}$$

with V_v the volume fraction of A and $\bar{V}(A')$ the average volume of objects A'. For a Boolean scheme of spheres of radius R, $\bar{V}(A') = 4/3.\pi.R^3$.

Let A_d be a Boolean scheme defined as the dilation of A by the ball $B(r)$,

$$A_d = A \oplus B(r) \tag{2}$$

This dilated Boolean scheme is equivalent to a Boolean scheme with a sphere of radius $R + r$, i.e. $\bar{V}(A'_d) = 4/3.\pi.(R + r)^3$. Let $V_{v,d}$ be the volume fraction of the Boolean scheme A_d defined as

$$1 - V_{v,d} = \exp(-\theta.\bar{V}(A'_d)) \tag{3}$$

Using (1) and the expressions of $\bar{V}(A')$ and $\bar{V}(A'_d)$ we can express $V_{v,d}$ as a function of V_v

$$\begin{aligned} 1 - V_{v,d} &= \exp\left(\ln(1 - V_v).\left(\frac{R + r}{R}\right)^3\right) \\ &= (1 - V_v)^\alpha \end{aligned} \tag{4}$$

where $\alpha = \left(\dfrac{R + r}{R}\right)^3$.

Henceforth a limit value of r that we called the critical radius r_c can be obtained when $V_{v,d}$ is equal to the critical percolation-threshold ρ_c.

$$1 - \rho_c = \exp\left(\ln(1 - V_v).\left(\frac{R + r_c}{R}\right)^3\right) \tag{5}$$

The critical radius r_c is then defined by

$$r_c = (\sqrt[3]{\beta} - 1).R \tag{6}$$

where $\beta = \dfrac{\ln(1 - \rho_c)}{\ln(1 - V_v)}$.

Assessment of the critical percolation-threshold

As in [1], [10], we consider that a realization percolates when there exists at least one connected component connecting two parallel faces of a representative cube. The critical percolation-threshold ρ_c is numerically computed in [1] by dichotomic search. Several set of $2N$ realizations of Boolean schemes are processed with different V_v. ρ_c is obtained as the volume fraction of objects when exactly N realizations percolate.

Our method avoids the dichotomic search and allows a time-saving trick. N realizations of Boolean scheme are generated and successive dilations applied on A' increase V_v. The 3D distance transform (see [12]) to which an increasing threshold is applied, allows these dilations. ρ_c is then computed without

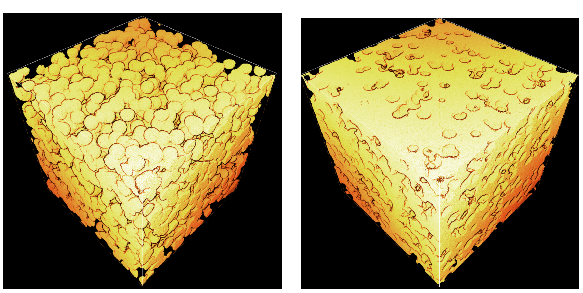
generation of new realizations with different V_v.
We assess ρ_c on 20 realizations of size 300^3 of a single-scale Boolean scheme of spheres with $V_v = 0.5$ and $R = 10$. We obtain a critical percolation-threshold value equal to 0.914 for the complementary set in close relationship with the reference value 0.946 numerically found in [13]. This discrepancy finds its origin in the low precision computation due to the small ratio: volume size/$(R+r)$(this ratio is equal to 30, whereas it is 400 in [13]).

Numerical computation of the reachable volume fraction

Our quantitative approach of the percolation allows the definition of new morphological descriptors. The computation process is described. N realizations of single-scale Boolean schemes of spheres with given V_v and R are generated. Let I be one of these realizations. We focused in the percolation of the complementary set I^c. We erode I^c by a spherical element with increasing radius r and the reachable volume fraction V_r is computed at each step. V_r is defined as the summation of the volume fraction of all connected components which percolate,

$$V_r = \sum_i V(CC_i)/V_T \tag{7}$$

where CC_i the i^{th} percolating connected component, $V(CC_i)$ its volume and V_T the total volume. The term "reachable" represents then the accessibility for spherical particle which looks for percolating through the porous network. The successive erosions, efficiently computed by means of a geodesic distance map D_g [12] (threshold of D_g), allow the simulation of a percolating sphere with increasing radius until r_c is reached. In practical the algorithm's end is defined by V_r equal to zero, the critical point is the coordinates which precede this "limit". The numerical r_c is the abscissa of this critical point.



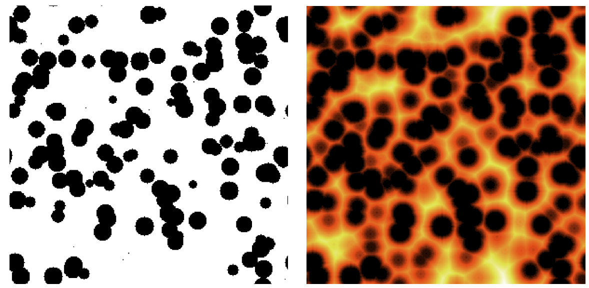
(a) (b)

Fig. 1: (a) Realization of a Boolean scheme of spheres with $R = 10$ and $V_v = 0.5$ and (b) its complementary set.

III. Results and Discussion

Single-scale Boolean scheme

First we assess the critical percolation-threshold ρ_c by increasing the volume fraction V_v on single-scale Boolean schemes of spheres. The reachable volume fraction V_r can be computed until r_c is reached in the vicinity of $\rho_c = 0.946$. We applied our descriptors on Boolean schemes of spheres with $V_v = 0.7$ and $R = 10$. The volumes generated have a size of 300^3. For an aesthetic purpose Boolean schemes of spheres with $V_v = 0.5$ and $R = 10$ are shown. Figure 1 presents a realization of such a model and 2D slices of I^c and distance map D_g used to calculate erosion are shown figure 2.



(a) (b)

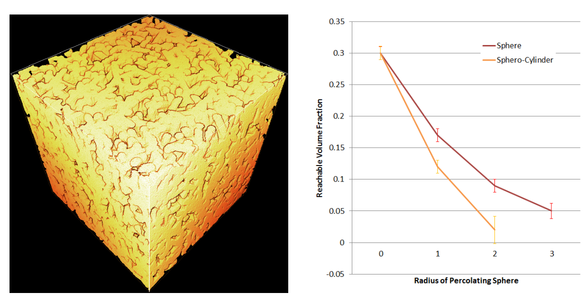
Fig. 2: (a) 2D slices of I^c and (b) of the geodesic distance map D_g for a realization with $R = 10$ and $V_v = 0.5$.

Computation of V_r as a function of r is presented in Table I. The third line presents the evolution of V_v and shows its increase until the vicinity of ρ_c.

r	0	1	2	3
V_r	0.30	0.16	0.09	0.05
V_v	0.70	0.78	0.85	0.91

TABLE I: Morphological descriptors of single-scale Boolean schemes of spheres with $V_v = 0.7$ $R = 10$.

Our morphological descriptors are then applied on single-scale Boolean schemes of sphero-cylinders. A sphero-cylinder is a cylinder with two hemispherical caps at each end, thus defined by two parameters L the length of the cylinder and R the radius for the hemispheres. Volume fraction V_v and average volume $\bar{V}(A')$ are assigned the same as the Boolean scheme of spheres. Figure 3 presents a 3D image of one realization and the comparison of the descriptors with the previous scheme of spheres.



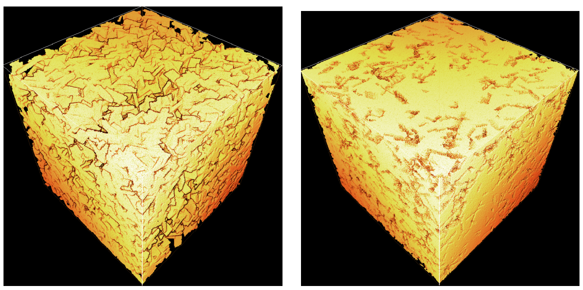
(a) (b)

Fig. 3: (a) Single-scale Boolean scheme realization of sphero-cylinders with $R = 5$, $L = 47$ and $V_v = 0.7$ and (b) the reachable volume fraction evolution for Boolean schemes of spheres ($V_v = 0.7$) (red) and sphero cylinders (yellow).

The critical radius r_c is equal to 2 and 3 for Boolean schemes of sphero-cylinders and spheres respectively. This difference results from the diameter of sphero-cylinders which is bigger than the one of spheres for a same volume. Here the diameter is defined as the maximal distance between two points of the object. Moreover the decrease of V_r for sphero-cylinder's case is more important than for sphere. Both descriptors discriminate the schemes.

Multi-scale Boolean scheme of aggregates of constant radius

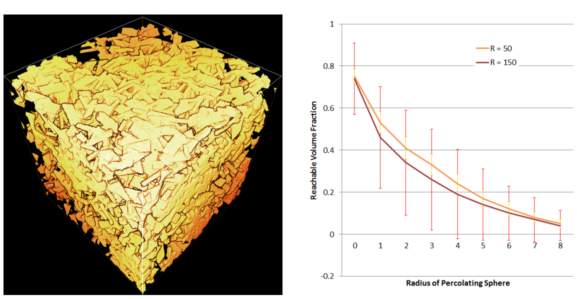
We applied our descriptors on complex multi-scale Boolean schemes of platelets' aggregates presented by Figure 4 which can be used to simulate digital microstructures of alumina catalysis supports [14].



(a) (b)

Fig. 4: (a) Multi-scale Boolean scheme of platelets with the radius of aggregate's spheres equals to 150 and (b) its complementary set.

This kind of Boolean scheme are defined by several parameters: shape of platelets, size of aggregates (R_{agg} radius of spheres), volume fraction of platelets inside (V_{agg}) and outside the aggregates. As seen previously the accessibility for an enlarging sphere is assessed and the reachable volume fraction V_r is computed for two schemes differing by one parameter, in this case R_{agg}. The first scheme presented Figure 4 is generated with $R_{agg} = 150$. The second one has a radius of aggregate's spheres equal to 50. We compute the assessments on $N = 20$ realizations for each scheme.



(a) (b)

Fig. 5: (a) Multi-scale Boolean scheme of platelets with radius of aggregate's spheres equals to 50 and (b) the reachable volume fraction evolution for radius of aggregate's spheres equal to 50 (red) and 150 (yellow).

The critical radius r_c is identical for both schemes and equal to 8 (abscissa of the critical point of both curves Figure 5). Nevertheless there is a noticeable difference in the evolution of V_r on the graph Figure 5. Here the scalar descriptor does not be enough to distinguish the structures and the vectorial description is necessary.

IV. Conclusion

We have presented an original approach to percolation which leads to new morphological descriptors. These descriptors allow the quantification of the volume accessibility of complementary set (here multi-scale Boolean schemes) according to specific percolating spheres with increasing radius. In a further work we will apply these new descriptors to the characterization of real porous lattices of catalysts.

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