

How does a patchy network affect the structure of invading percolation patterns?

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Abstract

Invasion percolation with trapping (TIP) is studied on two kinds of pore networks. The first class of them is the one generated through the dual site bond model [I. Kornhauser, R.J. Faccio, J.L. Riccardo, F. Rojas, A.M. Vidales, G. Zgrablich, Structure characterization of disordered porous media, *Fractals* 5 (3) (1997) 355–377; S. Cordero, I. Kornhauser, A. Dominguez, C. Felipe, J.M. Esparza, F. Rojas, R.H. López, A.M. Vidales, J.L. Riccardo, G. Zgrablich, Site–bond network modeling of disordered porous media, Part. Part. Syst. Charact. 21 (2004) 101–116] (DSBM). This model allows different strengths of correlations among the elements of the lattice in such a way that patches of sites and bonds with similar sizes are structured as correlations are set up. The typical size of these patches depends on the strength of correlations.

The other class is a set of networks with a chessboard-like structure, i.e., patches are the “black” and “white” squares of a chessboard. Each square is made with bonds of similar sizes sampled from the same bond distribution. Black squares have sites sampled from the lower half part of the site distribution and sites in white squares belong to the other half.

When a network is built, both models have the constraint imposed by a construction principle (CP) that forbids a bond to be greater than any of the sites to which it is connected. This is a common used assumption in modeling porous networks.

The aim of this paper is to find whether the global patchy structure is responsible of the patterns found in TIP, or it is the local constraint imposed by the CP, which prevails. To this end, we measure different quantities, such as fractal dimensions, trapped fluid island distributions and invaded volume ratio, among others.

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1. Introduction

Spatial correlations are most of the time present in real porous media, from geological formations to mesoporous catalyst supports. This natural fact makes transport processes features more attractive, although modeling becomes more complicated.

A great amount of work has been done to characterize these correlated structures and much is still lacking to do [2–6].

One of the underlying problems when modeling a transport-in porous-media process is the statement of a network model. Any assumption made in the model introduces approximations and/or simplifications to the real situation. Thus, it is crucial to establish which are the main parameters affecting the physics of

the problem under consideration in order to avoid unnecessary complications in describing it.

How does one introduce spatial correlations in a model of porous media and how will they affect the behavior of transport and reacting properties through the medium is a standing problem in many physicochemical applications. A great amount of these phenomena is related to the dynamical description that offers invasion percolation (IP) through disordered site–bond networks, i.e., the porous medium is represented by sites (pore bodies) and bonds (pore necks) arranged together in a particular lattice configuration [6–8].

It has been demonstrated [1,3,4,6] that the introduction of space correlations in the network of pores, affects the way in which invasion is performed. This fact is revealed by the change of fractal exponents in the scaling of transport quantities, among other features [3,6,9]. Many models have been used to introduce correlations in a porous medium and to analyze transport prop-

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erties in it [2–4]. Among these models, we have particularly worked with the DSBM and found interesting behavior. On the other hand, the study of transport properties on chessboard-like networks has captured the attention of researchers [10].

The common feature in DSBM and chessboard models is that the topography of the network presents “patches”, i.e., regions that are made by the assembly of elements (sites and connecting bonds) that have similar sizes (radii). In DSBM, those regions are characterized by a spatial correlation length, r_0 , which depends on the overlap, Ω , between site and bond distributions, as we will see in the next section. This feature, joint to the local constraint that says that the size of any bond in the network is at the most equal to the size of either of the sites it connects, brings on the generation of space correlations of different extent, depending on the radii density distributions of the lattice elements. In the case of a chessboard topography, the two kinds of square patches are made with sites of different size, as will be better explained below. Here, the local constraint that a bond is always smaller or at least equal to the sites connected to it also exists. In this last model, patches are imposed by the chessboard structure.

This work analyses the effect of the presence of patches on IP in two-dimensional networks. Our objective is to establish which of the two topographic features affects the more the IP patterns: local constraints (CP) that finally develop long range correlations conforming patches of extent r_0 , or it is just presence of regions of elements of different alternating sizes (chessboard “squares”) no matter what causes these topographic features.

In the next section, we will present the two model networks used in our study. Section 3 will show some IP features and quantities of our interest. Section 4 will explain the simulation algorithms employed. Section 5 will show results and conclusions.

2. DSBM and chessboard models

As briefly explained above, two models were chosen to study the effect of correlations on IP patterns.

The DSBM has been explained elsewhere [1,2] but here, we will give the main aspects which are needed to understand our purposes and results. The interested reader can get deeper details in previous papers [1,11–14].

Let $S(R)$ and $B(R)$ be the distribution functions associated with the site and bond size R , and $F_S(R)$ and $F_B(R)$ the corresponding probability density functions, such that

$$S(R) = \int_0^R F_S(R') dR'; \quad B(R) = \int_0^R F_B(R') dR' \quad (1)$$

where R' is the variable of integration. The way in which sites and bonds are connected to form the network is given by the joint probability density function, $F(R_S, R_B)$, of finding a site with size $R_S \in (R_S, R_S + dR_S)$ connected to a bond with size $R_B \in (R_B, R_B + dR_B)$. The two basic laws describing the DSBM are:

$$B(R) - S(R) \geq 0 \quad (2)$$

$$F(R_S, R_B) = 0 \quad \text{for } R_S < R_B \quad (3)$$

The second law is often called the CP because Eq. (3) implies a law of a local nature and expresses the fact that the size R_B of any bond cannot be bigger than that of the two connected sites. In this way, when the network is constructed, the sizes of sites and bonds that are joint together must follow this statement. If the joint probability function is expressed as

$$F(R_S, R_B) = F_S(R_S)F_B(R_B)\Phi(R_S, R_B) \quad (4)$$

Then, the correlation function Φ carries the information about the site–bond assignation procedure in the network. If we denote by Ω the overlapping area between the site and bond probability density functions, the function Φ has the following properties: (i) $\Phi_{\Omega \rightarrow 0}(R_S, R_B) = 1, \forall R_S, R_B$, meaning that in this limit sites and bonds are distributed completely at random, and (ii) $\Phi_{\Omega \rightarrow 1}(R_S, R_B) \propto \delta(R_S - R_B) \forall R_S, R_B$, sites and bonds group together in macroscopic patches, each having a value of R . Then, the overlapping Ω is the fundamental parameter describing the topology of the network in this model.

This behavior also suggests that Ω must be related to some *correlation length* (which would be a physically more meaningful parameter), characteristic of the decay of the spatial correlation function defined as

$$C(r) = \langle R_S(\vec{r}_0)R_S(\vec{r}_0 + \vec{r}) \rangle = \langle R_B(\vec{r}_0)R_B(\vec{r}_0 + \vec{r}) \rangle \quad (5)$$

In fact, it is expected that $C(r)$ decays approximately as $C(r) \approx \exp(-r/r_0)$ where r_0 is the correlation length (measured in lattice constants). Monte Carlo simulations have shown that the correlation length r_0 is related to the overlapping Ω through the relation [14]:

$$r_0 \approx \frac{2\Omega^2}{(1 - \Omega)^2} \quad (6)$$

We observed that $r_0 \rightarrow 0$ for $\Omega \rightarrow 0$ and $r_0 \rightarrow \infty$ for $\Omega \rightarrow 1$.

The problem of numerical generation of DSBM networks has been intensively investigated. We employ here the method presented in [13] for the Monte Carlo generation of such networks.

In Fig. 1, we show two characteristic square lattices generated through DSBM. The top network is uncorrelated, as the gray scale homogeneity indicates. The bottom one corresponds to a high degree of correlation. This fact is made evident by the different gray scale zones (patches) as a result of the self-organization of the elements in order to achieve the CP. Dark gray are patches with smaller sites and light gray patches are made of big sites. This topography introduces a border line through out the whole network, a feature that will be crucial when a fluid is trying to percolate in it. What is the real importance of this border line is one of the questions to answer in this work.

The chessboard model was defined as follows. A square site–bond network was simulated. Here, we also had two size density distributions, one for sites and the other for bonds. The bond distribution was always at the left of the one for sites. No overlapping area was allowed (see Fig. 2a). The coupling of sites and bonds followed the CP. The two characteristic square patches (“white” and “black” squares on a chessboard) were obtained by separating the density site distribution in two classes: those sites

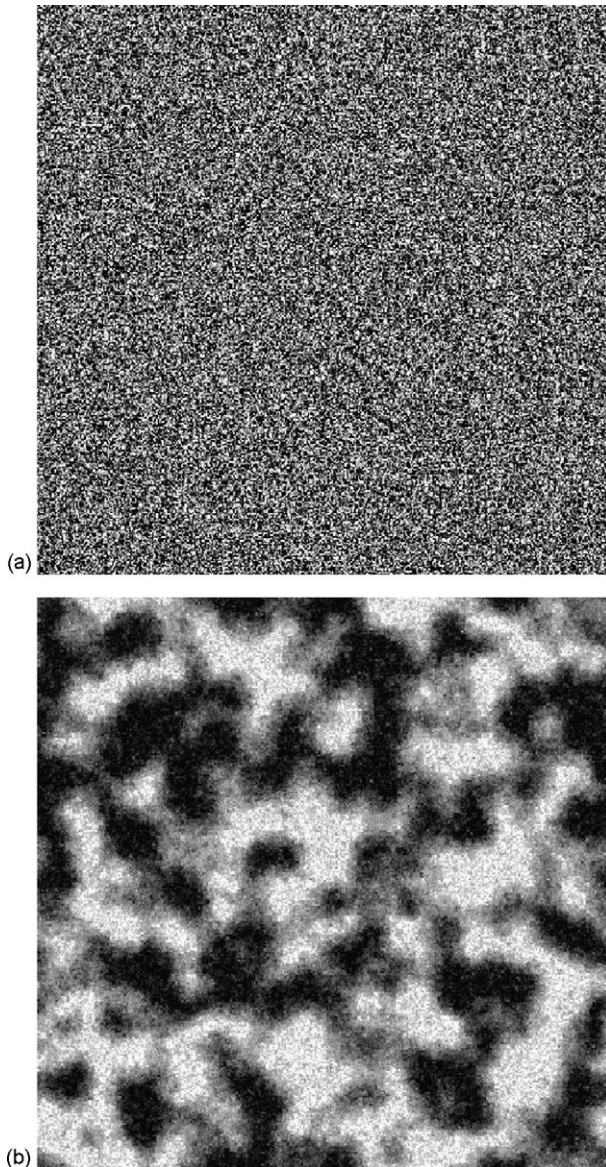


Fig. 1. Two characteristic square lattices generated through DSBM. The top network is uncorrelated ($\Omega=0$), as the gray scale homogeneity indicates. The bottom one corresponds to a high degree of correlation ($\Omega=0.9$). The gray scale used is explained in Fig. 2.

less than R_c and those greater than R_c , as shown in Fig. 2a. Bigger sites were chosen to form “white patches” and smaller ones to built “black patches”. Because there was no overlapping area among distributions, the assignment of bonds was easy to perform. Fig. 2b shows the appearance of the network once it was generated. Let l be the size of each of the patches and L is again the size of the network. In this way, dark gray squares (patches) are made of sites that are always smaller than the ones belonging to light gray squares. This fact introduces a border line that has to be overcome by the fluid in order to go from a “smaller sites” zone to a “bigger sites” one. How does this border line affect the passage of the percolating fluid through the system is another question to answer here.

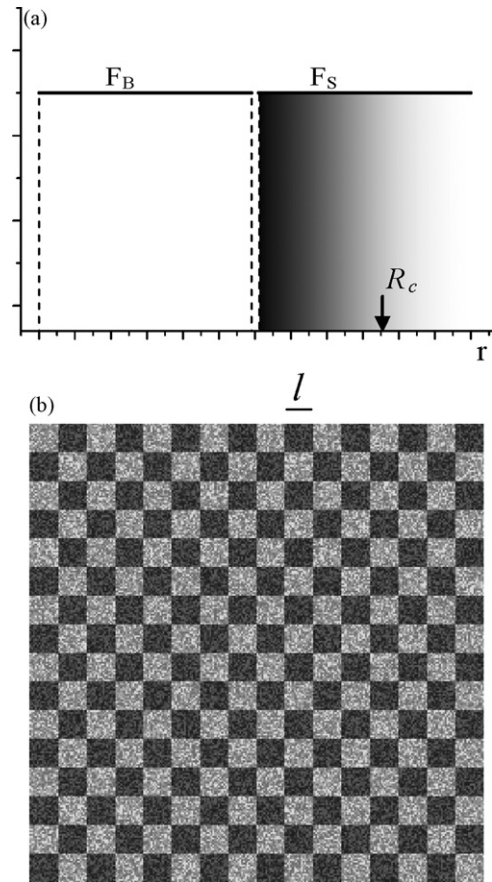


Fig. 2. (a) Bond and site distribution density functions. The gray scale for sites indicates their size. (b) Appearance of the network once it was generated. The size of each of the patches, l , is indicated.

3. Invasion percolation concepts

We used here the standard formalism of IP theory [15–17]. In particular, we simulated invasion patterns where the defending fluid was incompressible, thus, the formation of islands of the defending fluid surrounded by the invading one, might be present. In this way, we simulated TIP. The invader occupies the smallest site at the left side of the network and proceeds to invade the smallest neighbor linked to the already invaded site. Going on with this invasion algorithm, an invading irregular front is created. Each new invasion step is performed by checking the sizes of empty elements (sites or bonds) in contact with this front. The fluid always penetrates the smallest element at the frontier. As invasion proceeds, the defender “escapes” through the right side of the network. If the invader surrounds elements with defending fluid, “escape” is not possible and the surrounded fluid becomes trapped. In this way, an invasion cluster is developed that has fractal characteristics and, the first time this cluster touches the right side of the network we would say that it has percolated. This fact defines the so-called *percolation threshold*. To associate this process with a classical physical problem, let think about the displacement of one fluid by another one in a porous medium. When water is injected very slowly into a porous medium filled with oil, capillary forces dominates viscous ones (low Reynolds numbers). Thus, the dynamics is determined by the local pore

Table 1
Fractal dimension for several lattices

Lattice	z	D_f
Site (NTIP)		1.8959
Site (TIP)		
Hexagonal	3	1.831
Square	4	1.825
Triangular	6	1.89
Star	8	1.896

radius. Capillary forces are stronger at narrower pores: water displaces oil easier from the smallest available pore.

If one measures the fractal dimension, D_f , of the cluster at threshold stage, would find that $D_f = 1.82$ for a square lattice. If trapping is not allowed (compressible fluids, no trapping IP, NTIP) the value of D_f is a little bit higher, see Table 1 and Ref. [6].

Recently, Knackstedt et al. [6] found a non-universal behavior of IP in two-dimensional systems. It appears that D_f varies with

coordination number z for TIP. As z increases from four (square lattice) to eight (star lattice) the fractal dimension increases and approximates almost exactly to its value for NTIP, as shown in Table 1. They concluded that increasing connectivity causes trapping effects to decrease.

We will show below that not only connectivity, but also correlations, may cause non-universal behavior in D_f .

A question arising here is whether it is only the fractal dimension of the percolating cluster that changes or there are another dimensions that behave non-universal. One of them might be the random walk dimension D_w that relates the scaling behavior of the characteristic size λ of a random walk performed onto a fractal network after t time steps ($\lambda \propto t^{1/D_w}$). The other one could be the so-called spectral or fracton dimension, D_s , i.e., the one that surges whenever a physical quantity depends on the system's connectivity or branching properties [18]. It relates the probability $P(t)$ for a particle, performing a random walk onto a heterogeneous system, to be back at the origin at time t , i.e., $P(t) \propto t^{-D_s/2}$.

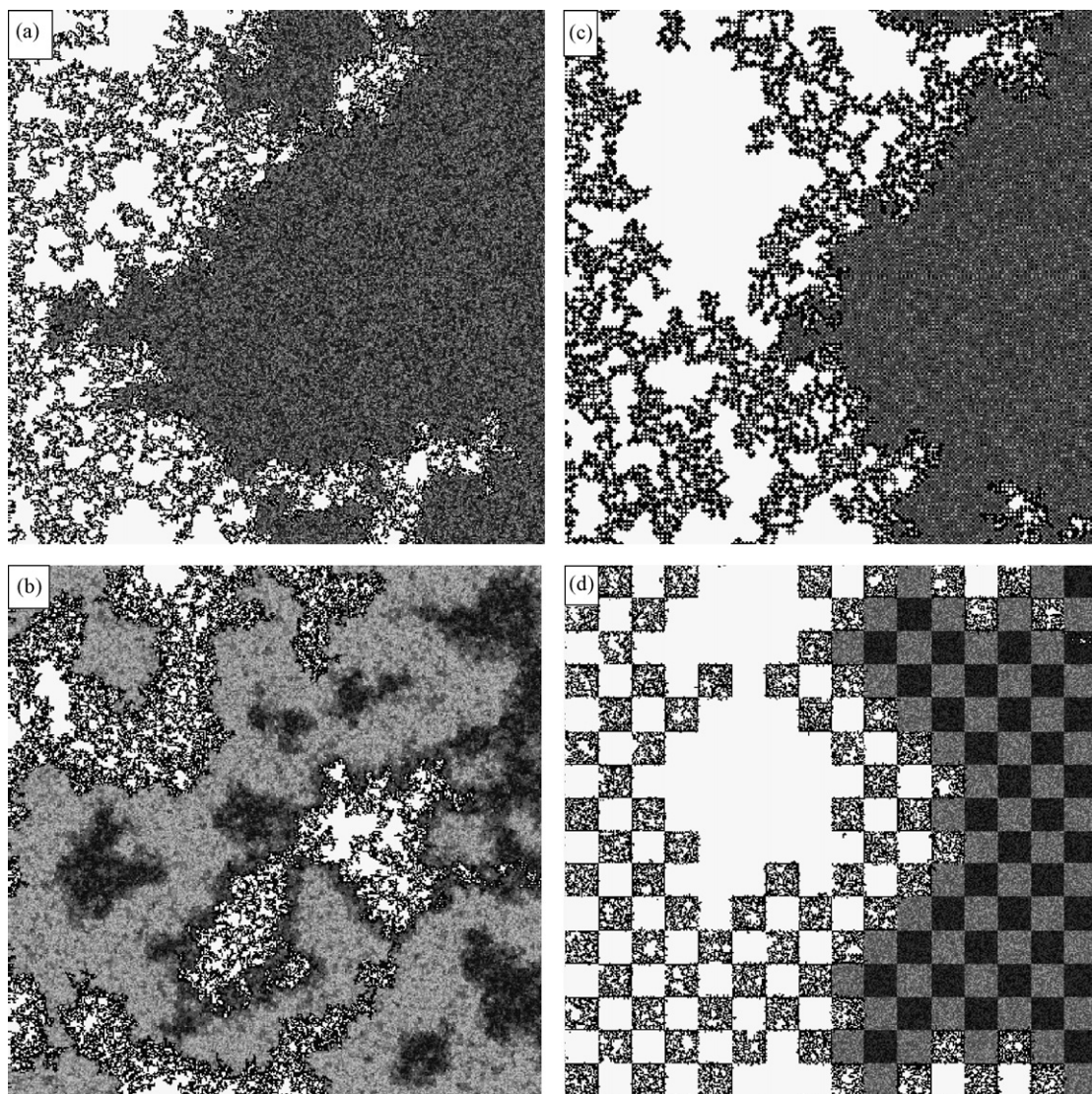


Fig. 3. Snapshots of the characteristic patterns appearing during the invasion process. In (a) DSBM, with patch sizes of 1 lattice unit ($\Omega = 0.5$); (b) DSBM, with patch sizes of 32 lattice units ($\Omega = 0.8$); (c) chessboard model patterns for $l = 1$; (d) chessboard model patterns for $l = 32$. Gray scale represents sizes as before.

4. Simulation algorithms

All the simulations involved averaging over several random walks on several different clusters. The clusters were grown to a size of 1,000,000 sites. The quantities shown in this section have been averaged over sets ranging from 1000 to 10,000 samples, depending on the size of the network ($32 < L < 1024$).

Assuming that a network corresponding to one of the two models explained previously has been generated, we proceed to simulate an invasion process. The network will have a characteristic patch size that will be related to the degree of correlation, in the case of DSBM, or will have to do with the size of the squares, l , in the case of the chessboard model.

The simulation algorithm employed for invasion is basically as follows:

- Initially, the network is filled with the defending fluid.
- The invading fluid advances through the network by invading the smallest element (even a site or bond) at the left edge of it.
- The list of all invaded sites and bonds at the interface between both fluids is actualized.

- The invading fluid proceeds by invading the smallest element belonging to that list.
- This procedure is repeated until the invaded elements (sites and bonds) form a cluster that “spans” the network, i.e., the cluster is able to connect the left edge of the lattice with its right one. This point is named “breakthrough stage”.
- Trapping of the defender can occur because incompressibility is assumed.

Fig. 3 shows snapshots of the characteristic patterns appearing during the invasion process. In (a) and (b), we see the invasion over networks generated by DSBM, with patch sizes of 1 and 32 lattice units, respectively. As indicated, these patch sizes correspond to an overlapping area $\Omega = 0.5$ and 0.8 , respectively. As explained earlier, Ω is the overlapping area between site and bond density distributions.

Snapshots (c) and (d) are the corresponding patterns for $l = 1$ and 32 in the chessboard model. The gray scale has the same meaning as before but it is worthy to make it clear that in all snapshots the gray scale for still not invaded sites was conserved; once a site was invaded, its color was turned to black and if it was

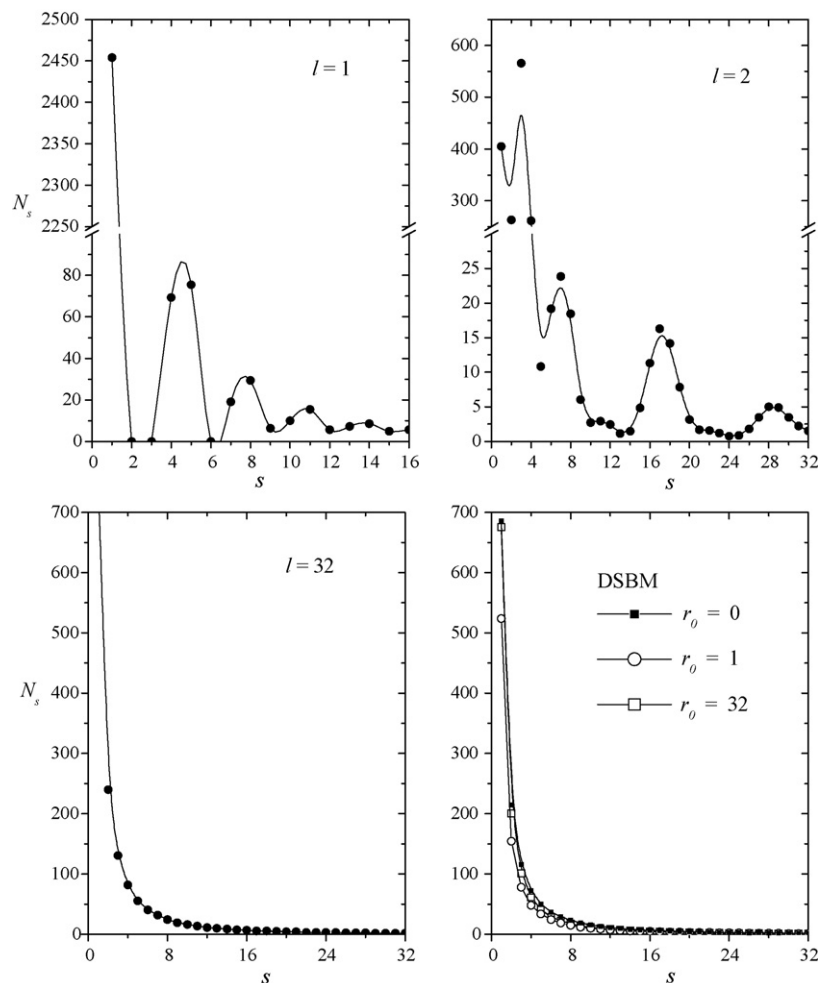


Fig. 4. Island distribution functions for the chessboard lattice and DSBM. Plots at the top (left and right) and left down corner correspond to the chessboard model with different l . The right-down plot corresponds to DSBM.

trapped it turned to white, thus, black points represent the invader fluid, white regions, the isolated defender.

5. Results and discussion

We have measured different quantities of interest. In Fig. 4, we show the island distribution functions for both models. In Fig. 4, right-down corner plot, we can appreciate that the island distribution for DSBM decays exponentially with the size of the islands, s , for all values of correlation strength. Here $r_0 = 0$ means that the invasion was performed on a random site–bond network. The case $r_0 = 1$ corresponds to a very low correlation (patches have a characteristic size of the order of one element). On the other hand, $r_0 = 32$ corresponds to a great strength of correlations, i.e., patches on the network have a characteristic size of 32 elements. Inside these patches, sites and bonds have very similar sizes among each other.

In the other three plots of Fig. 4, we clearly appreciate the chessboard effect on the creation of island of different sizes. The existence of a regular configuration for the distribution of site and bond sizes all over the network in “square” patches, makes some island sizes to be absent. This feature is more pronounced for low l . For example, for $l = 1$, islands of size two (two sites) can not appear because we need two nearest neighbors to be isolated in order to make them; this means (because $l = 1$) a “small class” site plus a “big class” site together. But this configuration is only possible if the fluid prefers to invade a big class site instead of a small class one. This, of course, is forbidden by the simulation rules themselves. The same reasoning can be followed for more complicated cases, explaining the absence of other sizes for islands in networks with $l = 1$ and other values of l . This feature in the shape of island distributions is distinctive of chessboard networks and is not present in DSBM ones.

Taking a look over the complete behavior of N_s versus s in the chessboard model shown in Fig. 4, one sees also an exponential decay for the number of island as s increases.

In order to calculate D_f , we made linear regressions on M versus L plots for the two models. M is the mass of the percolating cluster and L is the size of the network. For the chessboard model, data for $l = 1, 2$, and 16 were collected. For DSBM, networks with $r_0 = 0–32$ were inspected. Fig. 5a and b shows the results obtained for D_f for chessboard and DSBM, respectively. We also plot the values of D_w and D_s .

As previously pointed out [4], as correlation increases in DSBM networks, D_f changes from 1.82 (uncorrelated case) to 1.89 (fractal dimension for IP without trapping). On the other hand, D_f for chessboard networks seems to remain unchanged. This fact demonstrates that it is the presence of a local restriction, spread out all over the network in the form of patches, the responsible of a change in the fractal dimension of the percolating cluster. This patches are in some sense “connected” to each other by this local law and this makes it possible to change percolation properties like D_f . It is not just the presence of patches, without any connection among each other that favors the invasion.

For DSBM networks, considering the error in the measurements, it is not conceivable to establish a concrete dependence

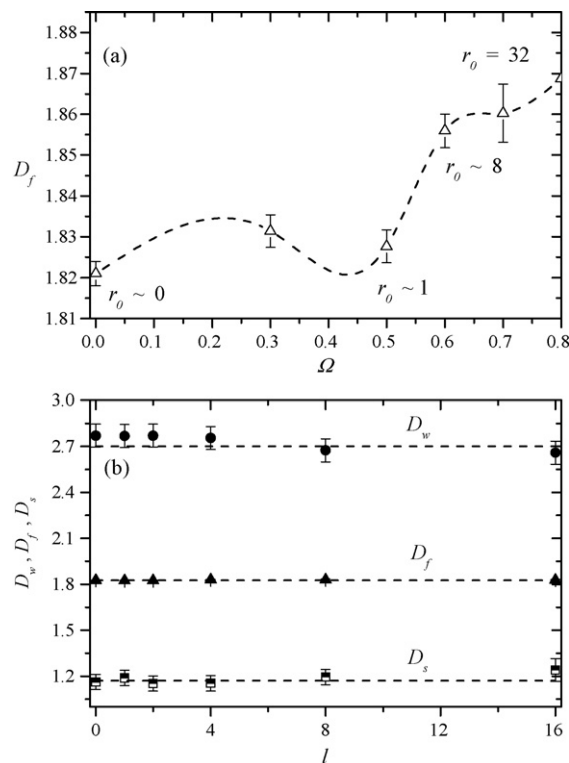


Fig. 5. (a) Fractal dimension for DSBM as a function of correlation degree. The extent of patches is indicated through the values of r_0 . (b) Dimensions D_w , D_f , D_s for the chessboard model as a function of the size of the patch, l . Dashed lines are to guide the eye.

of D_w on the spatial correlations, so we do not show plots of it. However, for low correlations it seems that the Alexander Orbach (AO) [19] conjecture is accomplished up to $\Omega = 0.7$ and, as correlations grow further, we observe a trend to lower values that have to be checked further. It is worth to remember that the AO conjecture received much attention for its intriguing relation between static and dynamic exponents. This conjecture based on numerical evidence was originally made for a percolating cluster. Imagine a random walk on a percolating cluster. The fractal dimensionality of the walk is, as explained above, D_w . If D_s is the fractal dimension of the percolating cluster AO conjecture states that the ‘fracton’ dimension D_s , given by $D_s = 2D_f/D_w$, has its mean field value $D_s = 4/3$ for any value of the Euclidian dimensionality D .

For chessboard networks, it can be concluded that the exponents are not affected by the presence of a strongly correlated surface and the AO is accomplished by the system [20].

Finally, Fig. 6 shows the behavior of the invaded volume, V_s , as a function of the degree of correlation and/or the size of the patches, for both models. For the case of DSBM there is a maximum for $r_0 \approx 2$ resembling the already observed non-monotonic behavior found in [9] where the creation rate of islands had a minimum for this extent of correlations. This is a particular aspect of correlated networks and is not present in the chessboard model where the behavior of the volume is monotonically decreased as the size of the patches is bigger. The existence of a competition between local correlations and global extent of the patches explains the presence of this maximum. The absence

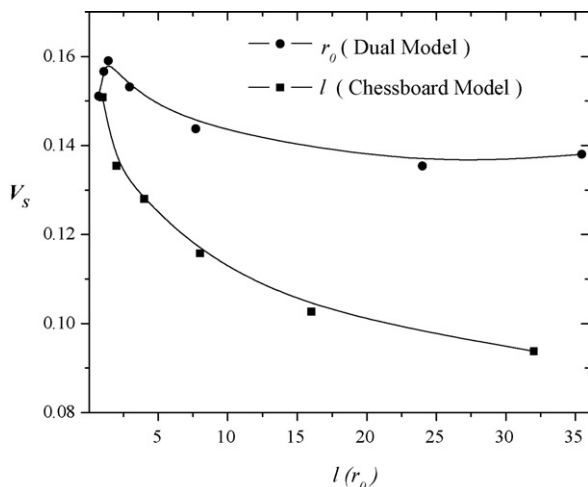


Fig. 6. Invaded volume, V_s , as a function of the degree of correlation and/or the size of the patches, for the two models.

of correlation spread in the chessboard model causes a continuous decrease of the invaded volume as bigger regions of porous space are avoided by the invader fluid.

6. Conclusions

6.1. For DSBM networks

Results indicate that the fractal dimension of the invasion sample-spanning cluster is non-universal for DSBM. It depends on correlation strength r_0 . The dynamic of the invasion process is affected by the presence of correlations and, as a direct consequence the fractal dimension of the invasion cluster changes.

The invaded volume fraction presents a maximum at low correlations. The existence of a competition between local correlations and global extent of the patches explains the presence of this maximum. The fact that local correlations spread out making network elements to join together to make patches, affects the filling performance for intermediate values of r_0 and does change percolation exponents.

6.2. For chessboard networks

Fractal dimension of sample-spanning clusters does not change with l . The same occurs for spectral dimension, D_s , and random walk dimension, D_w .

The dynamic of the invasion process is not affected by l . The qualitative behavior found for the filling process dynamics is in agreement with the quantitative independence of D_s and D_w . The invaded volume fraction decays considerably as l increases

due to the absence of correlation spread. Thus, the filling performance is lower than the corresponding one for DSBM.

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