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Role of Size Correlations in Fluid Displacement in Porous Solids†

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A 3-dimensional simulation of fluid displacement in a disordered porous solid is performed. The solid heterogeneities are characterized by two pore size distributions in the context of the dual site−bond model (DSBM). It is shown how invasion patterns and relevant quantities in invasion percolation are affected by the disordered porous matrix confirming and also contrasting previous results in 2-dimensional networks. Deeper understanding of the problem is achieved by allowing the presence of anisotropy in the porous space.

1. Introduction

Transport phenomena in porous materials have raised an ever increasing interest in the last two decades.[1−3] This is due to a wide variety of practical applications where these materials play a main role, most particularly in the oil industry, where the displacement of one fluid by another inside a porous reservoir is the primary mechanism by which hydrocarbons are produced. Considering this last process and from the viewpoint of modern physics, the evolution of the interface between two fluids provides a physical example of the phenomenon of pattern formation, i.e., viscous fingering and percolation features. The former occurs when a less viscous fluid displaces a more viscous one; the second, which will concern the present paper, occurs when the fluids are immiscible.

Browsing through the literature, we realized that most descriptions of a porous matrix suffer from the shortcomings of oversimplification or the use of too many adjustables parameters accounting for the complexity of the problem. This work presents a quite realistic representation of a porous space whose main characteristics are given just by one structural parameter concerning the degree of porous space correlations present in the medium. This is done by generating a 3-dimensional simple cubic network of sites and bonds which map, respectively, pore bodies and pore constrictions of the void space.

The disorder in the porous solid is achieved through the DSBM that will be briefly described in section 2. With the present model, it is also possible to introduce anisotropies in a straightforward way, which is also explained in the same section. An invasion percolation algorithm simulating fluid displacement is depicted in section 3, while, in section 4, the ways percolating quantities are affected by spatial correlations and by the presence of anisotropy in the size distribution of bonds are shown and discussed. Section 5 gives some remarks.

2. DSBM: Space Correlations and Anisotropy

Extensively described, the DSBM has proven to be very suitable to predict different kinds of physical processes occurring in disordered systems where correlations are present in variable extent.[2,4−6] Its main features are described elsewhere.[2,7−9] Here we will only show some of its main outstanding aspects and outcomings.

The sizes for the collection of sites and bonds representing pore bodies and necks in a simple cubic array are randomly sampled from two truncated Gaussian distributions (F_s, F_b) like those shown in Figure 1.

If we impose the restriction that each bond radius must be less than, or at most equal to, the radius of the smaller site to which it is connected (construction principle, CP), then the porous structure will depend not only on F_s and F_b but also on the way in which sites and bonds are assigned to each other.

This is completely specified by the joint probability density function, $F(R_s,R_b)$, of finding a site with size between R_s and $R_s + dR_s$ connected to a bond of size between R_b and $R_b + dR_b$, which can be written as:

$$F(R_s,R_b) = F_s(R_s)\, F_b(R_b)\, \Phi(R_s,R_b) \qquad (1)$$

where the correlation function $\Phi(R_s,R_b)$ carries information about the site−bond assignation procedure.

If we denote as Ω the overlapping area between the two probability density functions, and plot it against R, the function F has the following properties: (i) $\Phi_{\Omega\to 0}(R_s,R_b) = 1$, $\forall R_s R_b$, sites and bonds are distributed completely at random; (ii) $\Phi_{\Omega\to 1}(R_s,R_b) \propto \delta(R_s - R_b)$, $\forall R_s,R_b$, large patch limit.

It has already been shown that simulation of dual site−bond heterogeneous porous media becomes a difficult problem if there exists a high overlap between F_s and F_b (strong size correlation). The simulated density functions can be distorted, and any attempt to correct this distortion may give rise to spurious size correlations. There is strong evidence that the assignation of radii to sites and bonds

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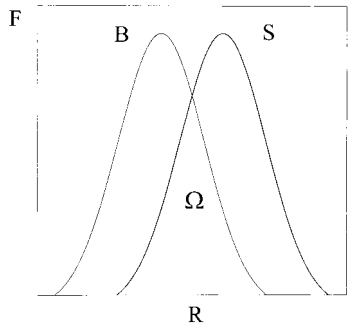

Figure 1. Site and bond size distributions showing the overlapping area Ω.

through a deterministic sequence of sites over the lattice can produce, as a consequence, strong anisotropy in the correlation between elements of the lattice.

We apply the powerful method developed by Riccardo et al.[9] to simulate a correlated porous network according to (1). This method provides a very easy way to apply Monte Carlo rules to reach statistical equilibrium for a wide variety of problems. For the case of DSBM, the metropolis algorithm can be readily applied. This means that, after a completely random assignment of the sizes of sites and bonds has been performed on the network, the necessary spatial rearrangements between the elements in order that the CP be obeyed, are carried out by attempting to exchange randomly selected pairs of sites (or bonds), not necessarily nearest neighbors, with a transition probability given by the metropolis rule on the basis of the joint probability $F(R_s,R_b)$. It is found[9] that this transition probability is 1 if the construction principle is obeyed as a result of the exchange and 0 if it is not.

The correlation function, Γ, between sizes of elements (sites or bonds) separated a distance, l, is found to decay exponentially as

$$\Gamma(l) \approx e^{-l/l_0} \qquad (2)$$

where l_0 is a characteristic correlation length (measured in lattice constants). This length has to do with the strength with which size correlations propagate through the structure and will of course be related to Ω with the extreme values 0 for Ω = 0 and ∞ for Ω = 1. An approximate relationship between the correlation length l_0 and Ω is $l_0 \sim \Omega/(1 - \Omega)$.

We will show below that the most interesting patterns occur for finite values of l_0 (intermediate Ω) and that the behavior for the extreme cases ($l_0 = 0$ or ∞) seems to converge with many common features.

Thus, the only relevant parameter needed to completely characterize the disorder in the medium (and the only one that will be varied in the present study) is the correlation extent, related either to l_0 or Ω.

One frequent feature concerning sedimentary porous structures is the presence of anisotropies.[11] These are generally present in one particular direction, due to the passage of ionic solutions and other fluids during the diagenetic process. This issue can easily be introduced in the present model by sampling the bonds in one particular direction (z, for example) from a different density distribution function with respect to the other ones (x,y); i.e., bonds in one direction are characterized by a different Ω

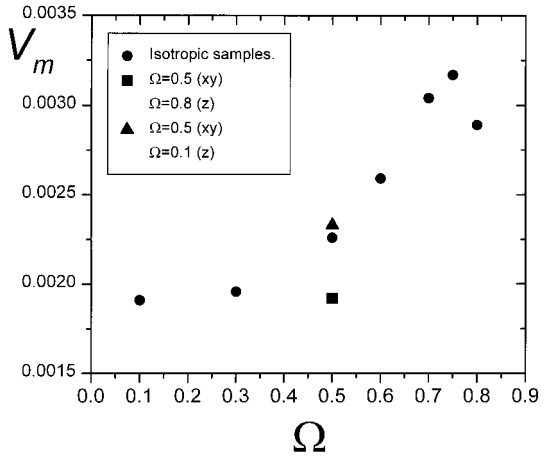

Figure 2. Mean front velocity as a function of the overlap.

than bonds belonging to the other ones. This fact will bring on important consequences in the invasion patterns as seen below.

In this way, cubic networks of sites and bonds are generated with edge size L (number of sites), with the desired Ω value. If the presence of anisotropy is required, another Ω value is selected for bonds in the z direction.

3. Invasion Algorithm

Assuming the whole network filled with an incompressible fluid, the displacing one begins the invasion through the smallest bond at the $z = 0$ face. The opposite face ($z = L$) is identified as the outlet face from which the displaced fluid escapes. At each time step the displacing fluid configuration grows by occupying the accessible element (site or bond) with the smallest sizes, i.e., scanning the interface for the smallest element in contact with the displacing fluid. Regions of the displaced fluid which becomes disconnected from the outlet face are trapped and cannot be invaded. The breakthrough state is reached when the invader touches the $z = L$ boundary for the first time. The process ends when none of the displaced fluid is connected to the outlet face (final stage). All the above rules constitute the so-called "invasion percolation with trapping" process. In our calculations the linear size of all the cubic networks was taken to be $L = 32$ sites.

4. Results and Discussion

All the quantities shown in this section have been averaged over a set of 100 samples. In the case of the snapshots, the selected patterns were those for the network whose percolation features were the closest to the corresponding averaged ones.

In Figure 2 the mean front velocity is defined as the rate L/N, where N is the number of invasion steps needed to reach the breakthrough. For the isotropic samples (black filled circles) an increasing trend is observed as Ω gets greater. A maximum is observed around Ω = 0.75 where the velocity begins to decrease. This is similar to the behavior found in 2-dimensional networks where V_m has also a maximum for intermediate values of Ω. Even though, in the present case, this maximum is achieved for a higher Ω than for 2-dimensions. This is due to the fact that the dependence of l_0 on Ω is expected to be different for Gaussian distributions than for uniform ones. The effect of correlations on V_m is clear looking at the corresponding snapshots, in Figure 3.

What happens when anisotropy is set up? Anisotropy was introduced by sampling the z bonds (bonds in z direction in the 3-dimensional network) from a distribution with $\Omega(z) = 0.8$ (squares in Figure 2) and $\Omega(z) = 0.1$

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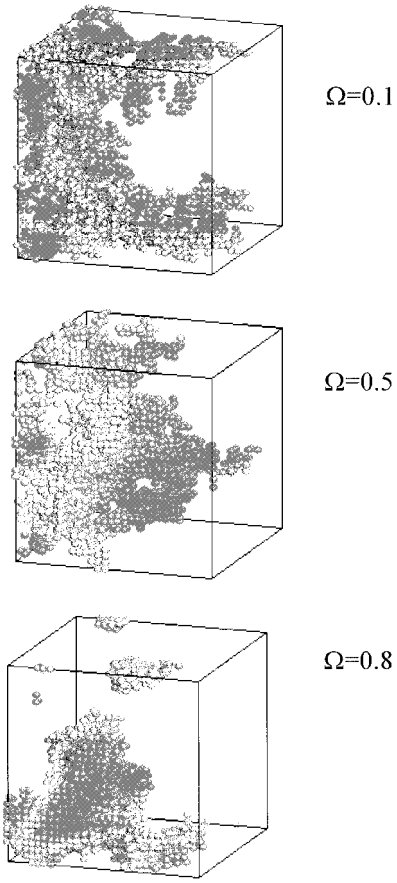

Figure 3. Snapshots of the invading fluid for different overlaps at the breakthrough state, for isotropic media.

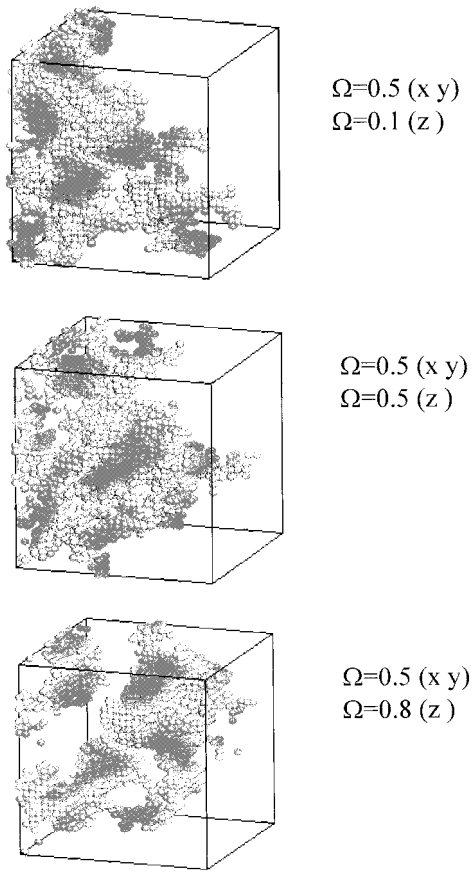

Figure 4. Snapshots of the invading fluid at the breakthrough state showing the effect of anisotropy.

(upright triangles in Figure 2) as the overlapping areas with respect to the site distribution. The bond distribution for x and y was kept the same as for the isotropic case, with $\Omega(x,y) = 0.5$ as the overlapping area with the same site distribution.

As seen in Figure 2, V_m is affected by the presence of anisotropy, i.e., is higher as $\Omega(z)$ is lower. This is easily explained if we consider that the probability for the invading front to get the smallest element (bonds in this case) is higher (lower) in the z direction than in the other two given that the z-bonds distribution is shifted to smaller (higher) size values with respect to the x−y distribution for the case $\Omega(z) = 0.1$ ($\Omega(z) = 0.8$). This effect is also shown in Figure 4.

In Figure 5, the number of islands of size between 2^k and 2^{k+1} are shown in a log−log plot.

The results for the isotropic samples are as expected. The stronger the correlations, the greater is the probability of finding large islands.[12] But an interesting feature is that, for anisotropic samples, one can see that the presence of large islands is mainly determined by the correlations in the z direction. When $\Omega = 0.8$, the number and size (up to 2^4) of islands in the isotropic sample (crosses) is of the same order as for an anisotropic one with $\Omega = 0.5$ in $x-y$ and $\Omega = 0.8$ in z direction (black squares) and almost 2 orders of magnitude grater than for the isotropic case $\Omega = 0.5$ (circles). Its counterpart (upright black triangles) shows that the anisotropic samples are the ones with fewer islands compared with both isotropic cases, $\Omega = 0.1$ and $\Omega = 0.5$. The conclusion is that at breakthrough the topology of the trapped space can be mapped with the

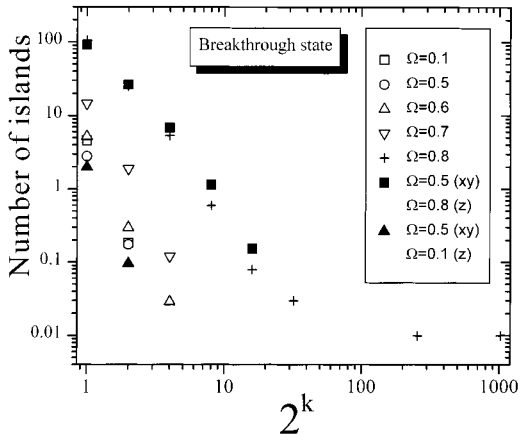

Figure 5. Size statistics of islands of trapped defender fluid at breakthrough state.

knowledge of the extent of correlations in the direction of flow advance.

Figure 6 shows the total number of steps, N_T, needed to reach the final stage. N_T has a maximum at $\Omega = 0.75$ as V_m has. Increase in correlations improve the displacing process up to a certain extent. An increase in Ω means that the "patches" (regions in the pore space where pores have nearly the same size) are greater and greater. Consequently, the development of the invasion inside each patch is performed as it were in a homogeneous pore space where invasion steps are done in all directions with the same probability; i.e., it is done in a less efficient way. This feature was also suspected in 2-dimensional networks, but at that time, statistical fluctuations at high Ω made it impossible to assume this. On the other hand,

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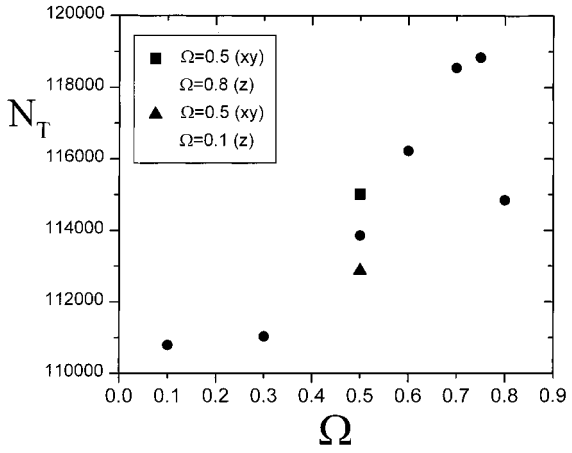

Figure 6. Total number of steps to reach the final invasion stage (completion) as a function of the overlap.

there is no minimum for N_T at intermediate Ω, as there was in the 2-dimensional counterpart.[12] In that work, the presence of this minimum was explained as the result of two competing effects: correlations enhance the invasion process (patches which are greater in size are bypassed), but when a patch is invaded, the invasion steps inside that patch grow as its size grows. This explained the behavior of V_m at breakthrough and *also* its behavior for the final stage quantities.

In the present 3-dimensional case, this effect seems not to be important at the final stage; i.e., given the greater connectivity in a 3-dimensional porous network, this short-range effect does not affect the total number of steps at modest Ω values.

Looking at the main features of the invasion patterns such as those shown in Figure 4, the invasion clusters which have Ω = 0.1 and 0.5 in the *z* direction seem to belong to the typical site invasion percolation ones observed in other models in 2 and 3 dimensions.[3,4,13] On the other hand, for the case Ω = 0.8 in the *z* direction, the cluster seems to "flat" its advancing surface, suggesting a change in the advancing front features such as that observed in the models of references.[3,4,13]

For anisotropic networks, N_T is greater for greater correlations in the *z*-direction, in contrast to the effect observed for V_m at breakthrough. This means that the anisotropy used here enhances the front velocity but does not affect the performance of the invasion. This is also clear in Figure 7a, where the final number of islands, N_{FI}, is plotted against Ω. The analysis of N_{FI} (Figure 7a) together with the final statistical classification of islands (Figure 7b) shows that the total number of trapped islands at low and high Ω are comparable except for the case of Ω = 0.8 where the number of medium size islands within the trapped regions decays considerably faster than the others. The minimum in N_{FI} corresponds to a decrease of approximately 20% compared with low and high Ω and is due principally to the smaller size island change (see Figure 7b).

The presence of anisotropies diminishes the number of islands of all sizes for the case Ω = 0.8 in the *z*-direction (black squares on Figure 7b) and makes the distribution practically indistinguishable from the isotropic case (Ω = 0.5) for anisotropies in the *z* direction with Ω = 0.1 (black upright triangles).

These effects on the invasion patterns due to the presence of anisotropy must be compared with the ones

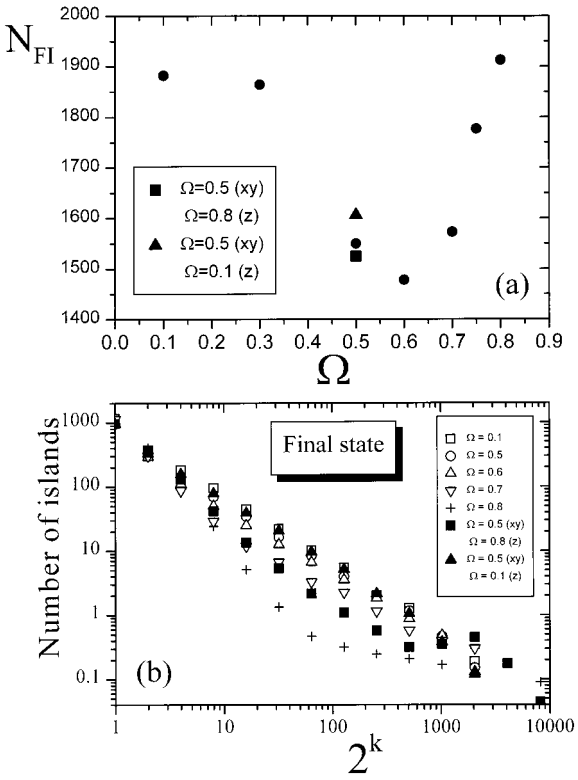

Figure 7. (a) Number of final islands of trapped defender fluid at completion as a function of the overlap. (b) Size statistics of islands of trapped defender fluid at completion.

observed in other processes such as diffusion through 3-dimensional porous networks where the parallel and transversal diffusion coefficients show a strong dependence on the way bond size distributions in each direction are set.[14]

The total invaded volume is not shown here because it displays the same qualitative behavior as the functional dependence of N_T on Ω, i.e., showing a maximum at Ω = 0.75 and with the same features when anisotropies are present.

5. Conclusions

The present study of invasion percolation properties on correlated 3-dimensional cibic lattices gives the following conclusions: (a) All quantities are shown to be affected by correlations in a non-monotonic way. Comparing 2-D and 3-D behaviors, different features are found due to the fact that in 3-D the effect of entrapment is lower. (b) The efficiency of the invasion process in terms of the amount of displaced fluid is maximized at moderately high correlations. After that, an increase in Ω implies that the patches are large enough that inside each one the invasion is performed as if were a homogeneous one, given the similarities in sizes inside the patch. (c) The presence of anisotropies in *z*-direction (direction of main advance) improves the invasion performance (black square in Figure 6) if they are stronger in that direction than in the others, but it produce a decrease in V_m (black square in Figure 2), and vice versa (black triangle in both figures).

To obtain a more complete understanding of the effects of correlation and anisotropy in 3-dimensional fluid displacements in porous media it is necessary to know the actual relation between l_0 and Ω for the distributions used here and also to know the fractal behavior of the spanning cluster at the breakthrough stage. Efforts are in progress in these two directions.

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