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Computer Model of a Porous Medium[1]

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A computer model has been set up to represent a porous medium. The basis for this model is a two-dimensional square network (100×100) of channels that have randomly assigned widths between the value of zero (closed) and the value of one (open, unrestricted flow). The channel width assignments have been made by a random selection from five different distributions: $f(q) = q$, $f(q) = \sin q$, $f(q) = \mathrm{erf}(q)$, $f(q) = 1 - \sin q$, and $f(q) = 1 - \mathrm{erf}(q)$. Diffusion of particles in the network has been studied by a random-walk procedure for each realization of the channel width assignments. The diffusivity is quite sensitive to the distribution of channel widths. The percolation properties of the networks obtained from the three most restrictive distributions have been investigated and the independent, linked clusters within the network have been determined. For cluster sizes that are less than the full width of the network, the network does not percolate and either the flow is not diffusive or the diffusivity is severely reduced. An approximate value for the percolation threshold has been determined in each case and the fractal dimension has been calculated also.

KEY WORDS: clusters; diffusivity; fractal dimension; percolation threshold; porous model; random channel widths; random walk.

1. INTRODUCTION

The field of porous media is attracting considerable attention from many areas of current interest such as enhanced oil recovery, nuclear and toxic waste storage, and filtration in environmental and biological systems, to name but a few. In view of the great variability of the medium, e.g., rock, for even one particular problem, experimental endeavors are necessarily inadequate and the need for predictive models is urgent.

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All the above-mentioned problems involve transport of material through a porous medium, and therefore, the method of molecular dynamical modeling suggests itself as a means of pursuing such investigations. To this end a model system must be set up that has the essential features of a porous medium, such as geometrical irregularity and connectivity, and its characteristics must be determined. This first step is the work described in this paper. For testing purposes, the model is set up in two dimensions. The extension to three dimensions is straightforward.

For five different irregular two-dimensional networks, the diffusivity has been determined by carrying out random walks on the network. An approximate percolation threshold has been obtained for three of these networks. For insight into the flow characteristics of the model, we have also determined the independent clusters in each network. Further, in view of evidence for porous media having fractal character over some length scale, we have estimated the fractal dimension from calculations of the radius of gyration of the clusters.

2. MODEL

A two-dimensional square network (100×100) is used as the basis for the model porous medium, the bonds in this network representing flow channels. An irregular structure is obtained by selecting channel width

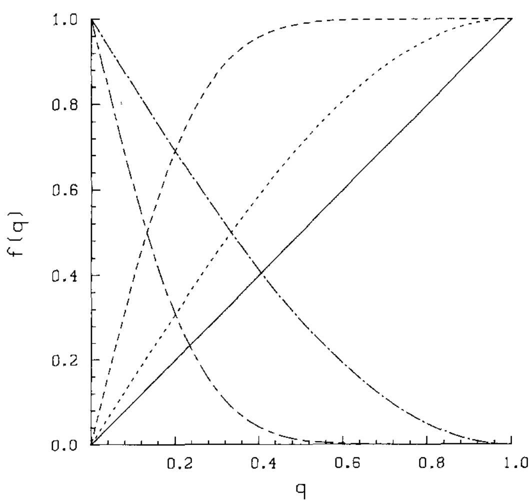

Fig. 1. Probability functions, $f(q)$. $f(q)=q$, ——; $f(q)=\sin q$, ---; $f(q)=\mathrm{erf}(q)$, ———; · $f(q)=1-\sin q$, —·—; $f(q)=1-\mathrm{erf}(q)$, —-—.

assignments from a distribution, $f(q)$, of random numbers, q. The channel is blocked when $f(q)=0$ and is fully open when $f(q)=1$. Irregular networks having a wide range of diffusivity have been realized by use of the distributions, (1) $f(q)=q$, (2) $f(q)=\sin q$, (3) $f(q)=\operatorname{erf}(q)$, (4) $f(q)=1-\sin q$, and (5) $f(q)=1-\operatorname{erf}(q)$, where $\operatorname{erf}(q)$ is the error function. These functions are shown in Fig. 1. Clearly, $f(q)=q$ yields a uniform distribution of channel widths, whereas for functions (2) and (3) the channel widths are weighted toward higher values and for functions (4) and (5) they are weighted toward lower values.

In order to determine the percolation threshold for each $f(q)$, a cutoff parameter, f_l, has been introduced such that all channel widths less than f_l are set to zero. The value of f_l is then increased, step by step, until at $f_l=f_p$, there is no significant diffusion.

3. CALCULATIONS

3.1. Diffusion

A random walk on each network has been carried out in the following way. (i) A random number determines which of the four possible directions ($\pm x$, $\pm y$) will be considered by the walker at position (i, j). If $0<q\leqslant 0.25$, we consider the x direction; if $0.25<q\leqslant 0.50$, the y direction; and so on. (ii) The random number is appropriately scaled and compared with the channel width in the selected direction. For example, if $0.25<q\leqslant 0.50$, then $q'=(q-0.25)\times 4$, and q' is compared with the channel width in the y direction. If the channel width is greater than q', the walker moves to the new position, $(i, j+1)$ in this example; otherwise, another random number is called and the process is repeated.

The mean square distance, $\langle r^2\rangle$, moved by a random walker on the network is calculated as a function of time (i.e., the number of steps taken in the random walk). Periodic boundary conditions are employed. The diffusivity, D, is given by the relation

$$\langle r^2\rangle = Dt \tag{1}$$

For the present calculation, adequate statistics obtain when all 10,000 network sites are used as the origin for a walker. In most cases, diffusion is established in less than 10,000 steps, but longer walks are necessary near the percolation threshold, where the diffusivity is very low.

3.2. Clusters

In a porous medium, the flow properties depend on the connectivity of the network, not just on the pore volume. For this reason, it is of interest to examine the networks we have generated for independent clusters of linked points. Those which extend across the full width of the network allow for flow; those from which a walker cannot escape are the so-called "dead ends." These dead-end clusters are ineffective in contributing to flow and are excluded from further consideration when dealing with a particular dynamical problem. Their presence gives rise to the phenomenological concept of "tortuosity," which describes the degree of difficulty in moving from one point to another in a medium of given porosity. Estimates of the tortuosity, δ, can be obtained from our results according to the relation [1],

$$D_\phi = D_0/\delta \tag{2}$$

where D_ϕ is the diffusivity in the network of porosity, ϕ, and D_0 is the diffusivity when f_1 is zero. The porosity is determined by the fraction of accessible sites in the network.

Another reason for interest in the independent clusters is that they provide a means of investigating the fractal character of the network. Once the clusters are defined, their radius of gyration, R_g, can be calculated and the fractal dimension, $\bar{d}$, estimated from the relation [2]

$$\ln N = \bar{d} \ln R_g \tag{3}$$

Values of $\bar{d}$ less than 2 indicate that the network does have a fractal character, at least over a length scale less than L, the total width of the network.

4. RESULTS

4.1. Diffusion

In Fig. 2, we show the results obtained for the average square distance moved, $\langle r^2 \rangle$, as a function of time, t, for all five networks. The networks are numbered (1)–(5), according to the distribution, $f(q)$, used to generate them (see Section 2). The diffusivity calculated for each case is listed in Table I in units of (network spacing)^2/step. The values, NT, given in this table are the duration of the walk in units of 1000 steps. The maximum distance moved by a walker, $r_{\max}$ (in units of network spacing), is also listed in Table I. Although we have investigated the percolation properties

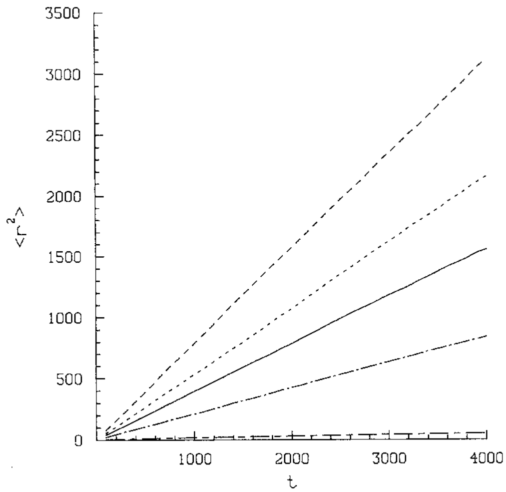

Fig. 2. Average square distance moved, $\langle r^2 \rangle$, versus time, t, for all networks. Network (1), ——; network (2), ---; network (3), ———; network (4), —·—; network (5), —-—. In all figures, distances are in units of network spacing and time is the number of random-walk steps.

Table I. Diffusivity and Parameters Characterizing Network

Network	f_1	$D \cdot 10^3$	NT	δ	ϕ	$\bar{d}$	r_{max}
(1)	0	386	4				131.83
	0.4	120	8	3.21	0.95		106.21
	0.5	240	12	15.4	0.66	1.91	78.31
	0.55	1.14	40	340	0.00	1.63	65.77
	0.6	0.065	12	5940	0.00	1.65	26.96
(2)	0	543	4				148.48
(3)	0	780	4				164.50
(4)	0	213	4				93.06
	0.3	8.78	20	24.3	0.34	1.70	79.98
	0.35	1.86	20	115	0.00	1.80	68.03
	0.4	0.058	20	3670	0.00	1.73	28.07
(5)	0	10.8	4				29.16
	0.015	2.41	20	4.48	0.33	1.62	47.07
	0.02	1.59	15	6.79	0.00	1.80	42.45
	0.025	0.854	15	1.26	0.00		30.48
	0.035	0.199	20	54.2	0.00	1.67	23.08
	0.04	0.173	20	62.5	0.00		21.40
	0.05	0.0391	20	276	0.00	1.55	18.87

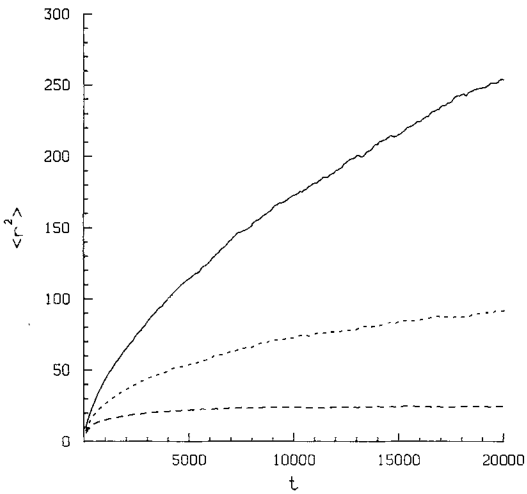

Fig. 3. Average square distance moved, $\langle r^2 \rangle$ versus time, t, for network (4): $f_l = 0.30$, ——; $f_l = 0.35$, ---; $f_l = 0.40$, — — —.

of networks (1), (4), and (5), because of space limitations, we now focus on network (4).

For a regular square lattice with bond percolation, the percolation threshold is $f_p = 0.5$. Therefore, we expect the threshold value for network (4) to be, by reference to Fig. 1, close to $f(0.5) = 0.3$. Figure 3 shows $\langle r^2 \rangle$ versus t for three values of f_l for network (4): $f_l = 0.30$, 0.35, and 0.40. The slope is quite small for $f_l = 0.35$, and we take this to be the approximate threshold value, f_p. For networks (1) and (5), $f_p = 0.55$ and 0.02, respectively. The diffusivity values for these cases and for several other values of f_l in networks (1) and (5) are given in Table I.

4.2. Clusters

In each of the cases listed in Table I, the independent linked clusters have been determined. In Fig. 4, we show the results for network (4), $f_l = 0.35$. For the sake of clarity, we have plotted only those clusters containing more than N_{min} particles [$N_{min} = 80$ for network (4)]. One cluster is almost large enough to span the full width, L, of the network, giving a small but nonzero diffusivity on the time scale of our calculations. Clearly, this network is very close to the percolation threshold.

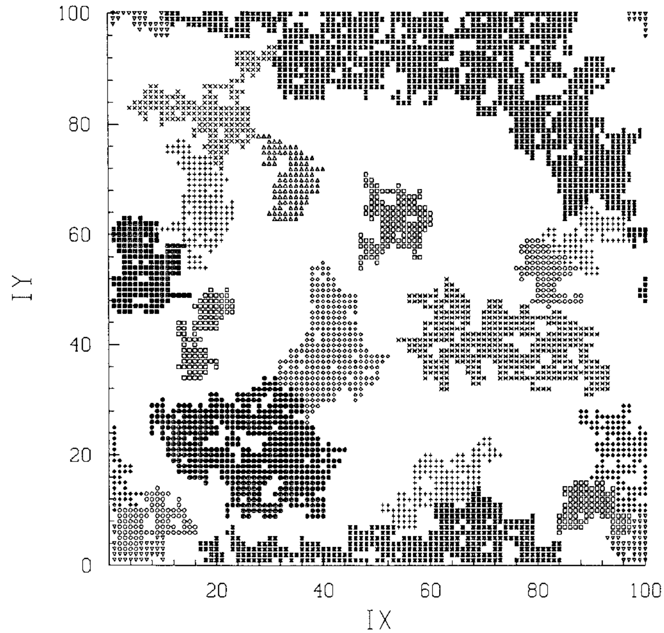

Fig. 4. Clusters for network (4): $f_1 = 0.35$, $N_{\text{min}} = 80$.

4.3. Fractal Dimension

The radius of gyration, R_g, has been calculated for each cluster. Then, for each network, the logarithm of the number of points in a cluster, $\ln N$, is plotted against $\ln R_g$. Figure 5 shows one such plot [for network (4), $f_1 = 0.35$]. The fractal dimension, obtained from the slope of these plots according to Eq. (3), is listed in Table I. In all cases, the slope is less than 2. In spite of the limited statistics, we conclude that there is some fractal character present in all these networks. Since percolation theory gives a value of 1.896 for the fractal dimension of a two-dimensional lattice at the percolation threshold [2], the lower values that we obtain indicate that those networks are below the percolation threshold.

4.4. Porosity and Tortuosity

In the networks that we have generated, one measure of the porosity is the fraction of bond widths that are set to zero, since this limits the accessibility of the sites. However, in measurements of porosity, it is the connected portions of the network that are important. Therefore, a better estimate of ϕ is given by the fraction of sites that are in clusters spanning

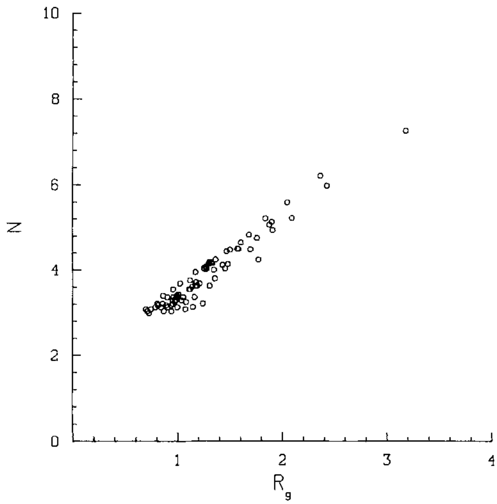

Fig. 5. Logarithmic plot of number of points in clusters v radius of gyration: network (4), $f_1 = 0.35$.

the network. With this definition, ϕ will be zero if there are no clusters large enough to span the network. The values obtained for ϕ are given in Table I.

As an additional descriptor of the system, the tortuosity parameter, δ, has been introduced to quantify the topological differences between networks with the same porosity. The tortuosity is related to the diffusivity according to Eq. (2). Values for δ, thus obtained, are also given in Table I.

5. SUMMARY

We have set up a model that has the essential features of a porous medium, i.e., it is an irregular network of connected pathways and dead-end regions. The model is characterized by the distribution function, $f(q)$, that is used to assign channel widths and by the number of blocked channels in the network (determined by the parameter, f_1). The diffusivity has been calculated for each combination $[f(q), f_1]$. In later work, f_1 will be used to control the size of particles that can pass through the network.

We have also investigated the topological features of the model by determining the linked clusters of points in each network. Flow can occur when a cluster spans the whole width of the network.

We have also determined the fractal dimension in each case and we conclude that the networks do, indeed, have some fractal character over the range, 100 lattice spacings, of our two-dimensional system.

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