Fractal Dimension in a Percolation Model of Fluid Displacement

In a recent Letter[1] Lenormand and Zarcone reported experimental measurement of the fractal dimension D for the invasion percolation (IP) process[2-4] at the percolation threshold p_c in two dimensions. The IP was proposed[2] to describe the process of the displacement of immiscible fluids in a porous medium. It is based on the dynamical growth of clusters of the invading phase along a path of least resistance. In one variation of the IP (which was investigated by Lenormand and Zarcone), the cluster of the invading phase *is not* allowed to grow into regions it has previously surrounded. This corresponds to the trapping of the blobs (clusters) of an incompressible fluid by the invading fluid. Monte Carlo simulations[4] have indicated that the fractal dimension of the growing cluster of the invading phase at p_c is about 1.82 in two dimensions, in contrast with $D=\frac{91}{48}\simeq 1.896$, for random percolation. Lenormand and Zarcone[1] displaced a wetting phase by a nonwetting one in a two-dimensional, transparent, etched network and found $1.8 < D < 1.83$, which is consistent with the Monte Carlo simulation result.[4] The purpose of this Comment is to draw attention to another percolation model for which the fractal dimension of the largest cluster (LC) at p_c appears to have the same values as that of IP. This model was developed recently[5] in an attempt to investigate the phenomenon of catalyst deactivation. In this problem gas molecules enter the pore space of the catalyst and react with the solid surface of it inside the pores. In parallel with the main reaction a side reaction also occurs that results in the deposition of an undesirable solid contaminant, which covers active sites, while simultaneously blocking part of the pore volume and decreasing its available surface area. Therefore, with process time more pores and sites are blocked and the catalyst gradually deactivates and a percolation threshold is reached. However, the process of pore blockage is not completely random: Smaller pores plug faster and once an island of partially blocked larger pores is surrounded by completely blocked (with no flow capacity) smaller pores, it can no longer be reached by the reactant and its blockage cannot be completed. We have performed Monte Carlo simulations of this process[5] with various pore-size distributions and reaction mechanisms and have found qualitative agreement with experimental data. To check the universality class of this model, we have estimated D at p_c by several methods. Note that unlike the random percolation where one can start the simulations at p_c, here we have to start from $p=1$. At any stage of the deactivation process, a pore has an effective (time-dependent) radius R_e which is given by[5] $R_e = R_0[1-\alpha g(t)/R_0]^{1/2}$, where R_0 is its radius at $t=0$, α is a parameter that measures the effective size of the deposit, and $g(t)$ is a function of the dimensionless time t which depends on the reaction mechanism, e.g., $g(t)=1-e^{-t}$ for a first-order reaction. Given an initial pore-size distribution and a reaction mechanism, one can, with the aid of this equation, keep track of the radii of all pores at any time and the isolated clusters of partially plugged pores (which are still considered to be active, although their flow capacity has decreased), until p_c is reached.

We used the standard finite-size scaling method with network sizes $L=40$, 60, 80, 100, and 130. At p_c the fraction X of pores in the LC scales with L as $X \sim L^{D-2}$, which yielded $D=1.81\pm 0.02$. Next, we used phenomenological renormalization of Monte Carlo data[6] and calculated X for several fractions of unblocked pores p for three L's: $L_1=80$, $L_2=100$, and $L_3=130$. The intersection of

$$\zeta_{L_1,L_2}(p)=\ln(X_{L_1}/X_{L_2})/\ln(L_1/L_2)$$

and ζ_{L_2,L_3} is $(p_c, 2-D)$ which yielded $D=1.82\pm 0.03$. Finally, we calculated the density-density correlation function, $C(r)=\sum_{r'}\rho(r')\rho(r+r')$, for the LC at p_c and $L=130$. One has $C(r)\sim r^{D-2}$, from which we obtained $D=1.82\pm 0.03$. We also used various pore-size distributions and reaction mechanisms with no change in results.

In conclusion, we have reported the fractal dimension of the LC in a modified percolation model which is different from that of random percolation, but is in agreement with that of IP reported by Lenormand and Zarcone.[1] Note that our model differs from the IP in several aspects, but the two models share one important feature: trapping of some clusters by others. This means that a percolation model, or possibly any growth process, in which some clusters may be trapped and remain untouched belongs to a different universality class from that of the model without the trapping rule. This is perhaps because the trapping rule has a global effect on the structure of the cluster and, as is known in other critical phenomena, a global effect is expected to change the universality class.

Muhammad Sahimi
Department of Chemical Engineering
University of Southern California
Los Angeles, California 90089

Received 5 June 1985
PACS numbers: 47.55.Mh, 05.70.Jk, 68.10.Cr

[1] R. Lenormand and C. Zarcone, Phys. Rev. Lett. **54**, 2226 (1985).

[2] R. Chandler, J. Koplik, K. Lerman, and J. F. Willemsen, J. Fluid Mech. **119**, 249 (1982).

[3] B. G. Nickel and D. Wilkinson, Phys. Rev. Lett. **51**, 71 (1983); J. F. Willemsen, Phys. Rev. Lett. **52**, 2197 (1984).

[4] D. Wilkinson and J. F. Willemsen, J. Phys. A **16**, 3365 (1983).

[5] M. Sahimi and T. T. Tsotsis, J. Catal. (to be published).

[6] M. N. Barber and W. Selke, J. Phys. A **15**, L617 (1982); M. Sahimi, J. Phys. A (to be published).

