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LETTER TO THE EDITOR

External surface of site percolation clusters in three dimensions

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Abstract. We study the external surface of site-percolation clusters in three dimensions by Monte Carlo simulations on a simple cubic lattice at $p = p_c = 0.3117$. Our results show that for all cluster sizes, s, more than 99.8% of the occupied sites are on the external surface. The number of unoccupied boundary sites t is found to obey $t/s = (1-p_c)/p_c + As^{-\psi}$ with $\psi = 0.54 = 1-\sigma$, in agreement with the prediction of a scaling argument. The same argument also predicts $\psi = 0.60$ in two dimensions and it is confirmed. The relevance of these results to dynamical percolation growth models is discussed.

Since the pioneering work of Leath (1976a, b), it has been well known that the surface-to-volume ratio of site-percolation clusters tends to a constant as the cluster size tends to infinity. In that work, the surface is measured by the total number of unoccupied sites (t) which are connected to the occupied cluster by a single nearest-neighbour (NN) bond and the cluster size is measured by the total number of occupied sites s. The surface-to-volume ratio at the percolation threshold p_c is given by

$$\frac{t}{s} = \frac{1-p_c}{p_c} + As^{-\psi} \tag{1}$$

where the exponent ψ was found to be approximately 0.52 in Monte Carlo simulations on a 2D square lattice. Thus the t/s ratio tends to an asymptotic constant determined solely by p_c.

In Leath's study, all surface sites internal or external to the cluster are included in the definition of t. In more recent years, because of the considerable interest in a variety of growth phenomena, one recognizes the importance of separating the internal surface sites from the external ones. The reason is simply that the external surface sites are often the only ones responsible for growth processes in physical systems. This feature is built into several dynamical percolation models, e.g., the invasion percolation model (see, e.g., Wilkinson and Willemsen 1983) for fluid displacement in porous media, the gradient percolation model for diffusion and invasion fronts (Sapoval *et al* 1985, Gouyet *et al* 1988) and the recently introduced Eden percolation model (Cao and Wong 1991) for heterogeneous reactions. In each of these cases, one finds that the *external perimeter* and the *hull* (see, e.g., Grossman and Aharony 1986, 1987 and references therein) of the ordinary percolation cluster play a crucial role in determining the fractal geometry of a moving front. The effects have also been observed in several fluid flow experiments (Shaw 1987, Hulin *et al* 1988, Birovljev *et al* 1991).

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The external perimeter and the hull are just slightly different definitions of the *external surface*. The former includes only those surface sites connected to the infinite unoccupied cluster by a single NN bond, whereas the latter allows a path of NN and NNN bonds to form such a connection. Both of these objects are now fairly well characterized in two dimensions. Computer simulations and exact solutions have shown that the external perimeter has a fractal dimension $D_e \approx \frac{4}{3}$ (Grossman and Aharony 1986, 1987) whereas the hull has a dimension of $D_h = \frac{7}{4}$ (Voss 1984, Saleur and Duplantier 1987). Both of these are different from the mass dimension $D_m \approx 1.89$. In contrast, we note that equation (1) implies that the total surface, which includes the internal surface sites, has the same fractal dimension as the mass. So the importance in distinguishing the external surface from the total surface is clear.

While the external perimeter and the hull have been well characterized in 2D, much less has been done for higher dimensions. The general expectation is that as the connected paths are much easier to form in higher dimensions, the probability for creating large interior voids should become much less. So one would expect the distinction between the external surface and the total surface to diminish with increasing spatial dimensions. There should be a *critical dimension* D_c above which the scaling behaviour of the external surface becomes the same as the total surface and the total mass. Most recently, Strenski *et al* (1991) reported a numerical study of the hull generated on a 3D bcc lattice. With an accuracy of about 1%, they found that $D_h \approx 2.52 \approx D_m$. This suggests that $D_c = 3$. However, given that D_h and D_m differ by only a few per cent in 2D and one expects the difference to be less in 3D, it is very difficult to conclude with certainty that the dimensions of the hull and the mass are truly identical. To provide a more stringent test, a numerical study of the external perimeter (surface) in 3D should prove useful because the external perimeter is a subset of the hull and so there is always a larger difference between the external surface and the total surface. For example, D_e is significantly lower than D_h and D_m in two dimensions. In other words, a determination of D_e in three dimensions would be a more sensitive indicator of how big a difference exists between the external surface and the total mass of the cluster. In the following, we describe our simulation results.

We carried out the simulations on a simple cubic lattice of size 200^3. Clusters were generated one at a time at $p = p_c = 0.3117$ using Leath's (1976a, b) kinetic percolation algorithm. The largest clusters have about 10^5 occupied sites. For each cluster, we identify the external surface sites (*e*-sites) as those occupied sites connected to the infinite unoccupied cluster by a single NN bond. The total number of such sites is called e and the number of unoccupied sites connected to them by a single NN bond is called t. The total number of bonds connecting between the two sets of sites is called b. The method for determining these numbers is quite straightforward. For each cluster, we first determined the maximal and minimal coordinates along the x, y and z directions and constructed an orthorhombic volume that just encloses the cluster completely. Each of the faces of this volume is a sheet of unoccupied sites external to the cluster. Starting from any site on one of these sheets, we identified its six nearest neighbours and checked if there is an occupied site among them. If so, then the centre-site is counted as an addition to the set of t-sites, its occupied neighbours are marked as e-sites and the connecting bonds between the two are marked as the b-bonds. For each of the unoccupied neighbours, we repeated the same checking and marking procedures of their NN sites. In other words, for each site that was checked, new external unoccupied sites were identified for further checking until all such sites were exhausted. Since only NN sites are checked at each step, none of the interior sites,

whether occupied or unoccupied, can enter into the counting of t, e and b. In addition, by marking every site when it was first checked, there was no possibility of double-checking or over-counting in these quantities.

The ratios e/s, t/s and b/s were determined for each cluster and averaged over a total of about 20 000 clusters. The dependence of these ratios on the cluster size s is shown in figure 1. For the e/s ratio, we note that it starts at 1 for $s=1$ and remains almost unchanged with increasing s. For $s>100$, we estimate that it has a constant value of 0.9984 (2), which means that more than 99.8% of the occupied sites are on the external surface. Although one might have anticipated the scaling behaviour of the external surface to be the same as the mass of the cluster, this very high percentage of external surface sites is noteworthy. It is a very strong indication that the external surface has the same fractal dimension as the mass and the total surface. Furthermore, since the external surface is a subset of the hull and the hull is a subset of the mass and the total surface, there is little doubt that the hull must also have the same fractal dimension, in agreement with the study of Strenski *et al* (1991). These results are strong evidence that $D_c=3$.

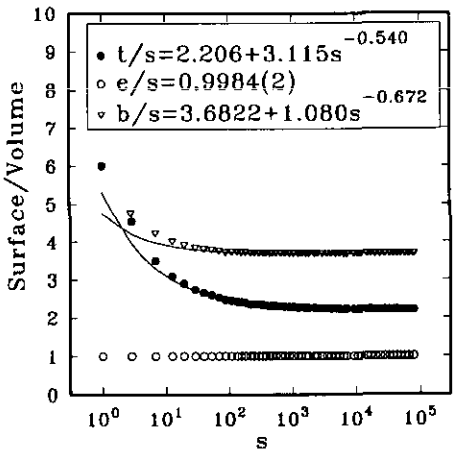

Figure 1. Surface/volume ratios for the external surface of clusters with occupied sites (s) up to 10^5. e/s measures the number of occupied sites on the external surface, t/s measures the number of unoccupied sites on the external surface, and b/s measures the number of bonds between the two sets of sites.

Since there is little difference between the external surface and the total surface in 3D, we would expect equation (1) to be valid for the t/s ratio of the external surface. Indeed, we find that our t/s data tend to a constant value of 2.206 for large s while equation (1) predicts a value of 2.208 for the total surface with $p_c=0.3117$. A least-squares fit of the data for $s>100$ gives $\psi=0.54$. This result is shown in figure 2 and it can be readily understood from scaling expressions given by Stauffer (1985) (see equations 33 and 44, figure 13 and table 2). Stauffer restated Leath's argument for the t/s ratio in terms of the cluster number n_s which is defined as the number of s-clusters per site (i.e., on a sample of L^d sites, one finds on average $L^d n_s$ clusters with s sites). For arbitrary p, the expression given by Stauffer is

$$\frac{t}{s}=\frac{1-p}{p}-(1-p)\frac{\mathrm{d}\log(n_s)}{\mathrm{d}p}. \tag{2}$$

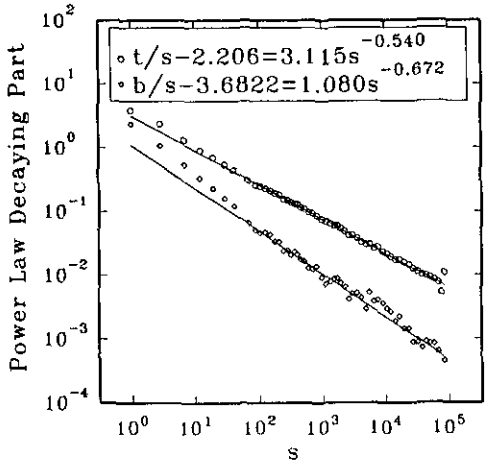

Figure 2. For percolation clusters generated on a simple cubic lattice at p_c, a least-squares fit of the t/s against s data to equation (1) shows that the region with $s > 100$ is well described by an exponent $\psi = 0.54$, in agreement with a scaling prediction. A similar fit for the b/s data results in an exponent of 0.67 which may be purely empirical.

Near the threshold p_c, n_s is expected to follow a scaling behaviour

$$n_s(p) = s^{-\tau} f[(p - p_c)s^{-\sigma}] \tag{3}$$

for large s, where f is a scaling function. Substituting equation (3) into (2) immediately yields equation (1) with $\psi = 1 - \sigma$ and $A = (1 - p_c)f'(0)/f(0)$. Stauffer's numerical data show that $f'(0) < 0$, so A is positive constant. The exponent σ is related to the other critical exponents by $\sigma = 1/(\beta + \gamma) = 1/(d\nu - \beta)$. The values tabulated by Stauffer give $\sigma = 0.45$ in 3D, which implies $\psi = 0.55$. Our result of $\psi = 0.54$ is in excellent agreement with this prediction.

It is interesting to note that Leath's 2D simulation is actually in slight disagreement with the above scaling prediction. According to Stauffer, $\sigma = \frac{36}{91} \approx 0.40$ in two dimensions, so $\psi \approx 0.60$. This value is a little larger than Leath's result of $\psi \approx 0.52$. The difference may be attributed to the fact that Leath's simulation was limited to a cluster size of $s \approx 1000$ which may not be large enough to reveal the asymptotic behaviour, because the external perimeter in 2D has a different scaling behaviour and it contributes most significantly to the total perimeter for small clusters. To confirm this, we repeated the simulation for a 2D square lattice for cluster size up to about $s \approx 10^5$. The t/s against s data are shown in figure 3. A least-squares fit of the data for $s > 300$ gives $\psi = 0.60$, in agreement with the scaling prediction.

For the number of bonds on the external surface, we find that the b/s data in figure 1 approach a constant value of 3.68 for large s. This value is remarkably close to 4 which is the value for a straight line of connected sites and it also shows how highly exposed the percolation clusters are in three dimensions. An attempt to fit the b/s ratio by an expression similar to equation (1) is shown in figure 2. The data with $s > 100$ may be described by an exponent of 0.67. We do not know of a simple explanation for this apparently larger exponent other than the fact that the data quality is not as good and the fit is less convincing.

In summary, we have found that the percolation clusters generated on a simple cubic lattice at p_c have over 99.8% of their occupied sites on the external surface and

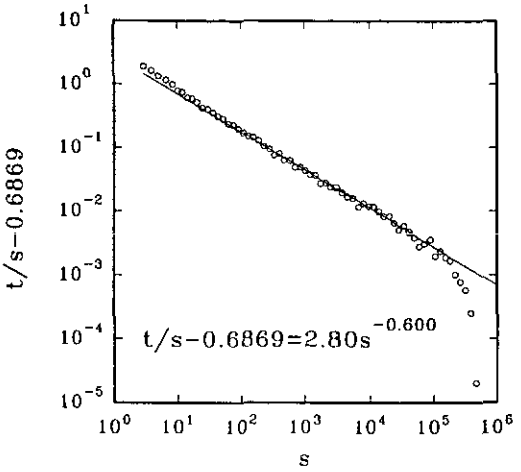

Figure 3. For percolation clusters generated on a 2D square lattice at p_c, the t/s ratio for the total surface also obeys equation (1) with $\psi = 0.60$. The range of s used in the fit is between 300 and 10^5. This result is also in agreement with the scaling prediction.

the t/s ratio is well described by equation (1). These results are strong evidence that the scaling behaviour of the external surface is the same as that of the total mass of the clusters in three dimensions, i.e., $D_c = 3$. If any difference (such as a logarithmic correction) does exist, it is certainly beyond the detection limit of a numerical study such as ours. The fact that the external and the mass have the same fractal dimension has some interesting implications. First, we note that the mass dimension D_m is about 2.5 in 3D, this may explain in part why fractal surfaces with dimensions around 2.5 seem to be ubiquitous among a wide variety of physical systems (see, e.g., Hulin *et al* 1988, Keefer and Schaefer 1986, Krohn and Thompson 1986, Schmidt 1989, Wong *et al* 1986). Second, we note that the Eden percolation model for heterogeneous reactions (Cao and Wong 1991) allows blocking particles larger than the growing ones. This may enhance the probability for creating interior voids and lead to a different behaviour for the surface. Further studies are required to clarify these possibilities.

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