Percolation with trapping

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Received 29 October 1985, in final form 17 February 1986

Abstract. A novel form of percolation is considered which is motivated by models of the displacement of one fluid by another from a porous medium. The physical idea is that if the displaced phase is incompressible, then regions of it which are surrounded by the displacing fluid become 'trapped' and cannot subsequently be invaded. We thus consider a new percolation process, 'percolation with trapping', in which one species (the displaced fluid) starts out at occupation fraction p = 1, but as p decreases only the infinite (connected) cluster is depleted; the finite (disconnected) clusters remain the same as when they are first detached from the infinite cluster. It is argued that the critical behaviour of percolation with trapping can be understood in terms of ordinary percolation exponents. In particular, the size distribution of the finite clusters at the end of the process has the same power law behaviour as in ordinary percolation. Relations with the process of invasion percolation are discussed.

1. Introduction

When one fluid displaces another from a porous medium and the fluids are immiscible, the configurations adopted by the fluids are often determined entirely by surface tension effects. This has led many authors to consider immiscible displacement in terms of percolation concepts (Melrose and Brandner 1974, de Gennes and Guyon 1978, Lenormand and Bories 1980, Larson et al 1981, Larson and Morrow 1981, Chandler et al 1982, Wilkinson and Willemsen 1983, Wilkinson 1985). However, the displacement process is not totally analogous to standard percolation theory for several reasons. The purpose of this paper is to investigate the differences which arise due to the fact that the displaced phase is incompressible.

To this end we have developed a new form of percolation which we call 'percolation with trapping'. This process is defined and analysed theoretically in § 2, where we present arguments that its critical behaviour may be understood in terms of that of ordinary percolation. In § 3, we present Monte Carlo simulation results supporting these arguments. Section 4 contains a discussion of the results, and the appendix lists certain definitions of percolation exponents which are used throughout the paper. The remainder of this introduction is concerned with the physical motivation for our model and may be skipped by the reader if desired.

When two immiscible fluids are present in a porous medium, the interface between the fluids is broken up into individual menisci which meet the pore walls with a contact angle determined by the three pairwise interfacial tensions between the two fluids and the solid. The fluid in which this contact angle is less than 90° is termed the wetting fluid and the other the non-wetting fluid. When the displacing fluid is the wetting

(non-wetting) fluid the process is called imbibition (drainage). Let us define the capillary pressure $p_{\rm cap}$ to be the pressure difference between the non-wetting and wetting phases:

$$p_{\rm cap} = p_{\rm nw} - p_{\rm w}. \tag{1.1}$$

This quantity should be thought of as an externally controlled macroscopic variable. If the flow rate is low enough, then at any value of the capillary pressure the system may be considered to be in capillary equilibrium, i.e. the menisci between the two fluids adopt configurations such that the interfacial pressure drop due to their curvature exactly balances the capillary pressure. In the course of the displacement, the capillary pressure gradually changes (in imbibition the capillary pressure decreases and in drainage it increases). As this happens, the menisci adjust their curvature accordingly, but from time to time a meniscus is unable to do this and jumps suddenly to some different configuration. This sudden motion is called a Haines jump (Haines 1930). Thus there are some parts of the pore space which fill with the wetting fluid (in imbibition) or the non-wetting fluid (in drainage) not gradually but suddenly, when the capillary pressure drops below, or rises above, some critical value. If the connectedness of one (or both) of the phases is controlled by these events we are led to a percolation picture of the process in which the occupation fraction of percolation is in one-to-one correspondence with the capillary pressure, i.e. at a given capillary pressure a certain fraction of these events can take place.

Let us imagine the porous medium to be a network of pores (sites) connected by narrower throats (bonds). In the fluid displacement problem there is a variety of possible jump events, some of which it is natural to assign to the sites of the lattice, and some to the bonds. For simplicity we will assign the events to the sites. To emphasise the generality of the phenomenon, we refer to the displacing fluid as the invader and the displaced fluid as the defender. A simple model of the invasion process on a given lattice structure is the following (Chandler et al 1982, Wilkinson and Willemsen 1983).

- (1) Identify a source from which the invader grows and a sink from which the defender escapes. These should be chosen to suit the physical situation; for example, the source and the sink might be opposite sides (faces) of the lattice. Initially all sites are occupied by the defender, except those identified as the source.
- (2) Assign a random number at each site (in the fluid displacement problem this represents the pressure at which the site will fill with the displacing fluid).
- (3) At each step, the invader cluster grows by occupying the available site with the smallest random number.
- (4) Regions of the defender which become disconnected from the sink are 'trapped' and cannot be subsequently invaded.
- (5) The process ends when all remaining defender occupied sites are disconnected from the sink.

We call the above process 'invasion percolation with trapping'. As in ordinary percolation there are two percolation thresholds, the first when the invader percolates (reaches the sink), and the second when the defender ceases to percolate (becomes disconnected from the sink). However, the above rules differ from those of ordinary percolation in two important ways.

(a) The invader grows only in a single cluster along a path of least resistance. This feature alone we will call invasion percolation. This is unlike ordinary percolation in which both species form many disconnected clusters.

(b) The defender can only be removed from the connected ('infinite') cluster and not from the disconnected ('finite') clusters. This feature alone we will call percolation with trapping. Again this is different from ordinary percolation in which both the infinite and finite defender clusters are modified as the defender occupation fraction is decreased.

These two differences are related to the connectedness properties of the two phases—difference (a) is related to the connectedness of the invader, and difference (b) to that of the defender. There is considerable Monte Carlo evidence that for planar two-dimensional lattices the combination of these two effects changes the universality class from that of ordinary percolation (Chandler et al 1982, Wilkinson and Willemsen 1983). This is apparently due to the fact that the two percolation thresholds get 'pushed together'—as soon as the invader percolates, the defender becomes disconnected. However, in three dimensions, the two thresholds are separated as in ordinary percolation, and it has been suggested that the critical behaviour of invasion percolation with trapping can be related to that of ordinary percolation (Wilkinson 1984).

In an attempt to separate the role of the above two effects, invasion percolation without trapping has been studied both by Monte Carlo simulation in two and three dimensions (Wilkinson and Barsony 1984), and by exact solution on the Cayley tree (Nickel and Wilkinson 1983). Some rigorous general results have also been obtained (Chayes et al 1985). The geometry considered in these papers was injection of the invader from a point into an infinite medium. Although invasion percolation is purely a kinetic growth process, the results of these papers strongly suggest that it is in some sense in the same universality class as ordinary percolation. In particular, the fractal dimension of the cluster appears to be the same as that of ordinary percolation clusters at threshold.

The purpose of the present paper is to investigate the effect of the trapping mechanism in isolation. Thus in the next section we introduce a process called 'percolation with trapping' which contains the trapping feature of invasion percolation with trapping but not the invasion feature.

2. Percolation with trapping

In this section we define and consider percolation with trapping for an infinite system. This is defined as follows.

- (1) We identify one species, the defender, which is initially at occupation fraction p=1, and which is gradually displaced by the other species, the invader. However, as we decrease the defender occupation fraction the invader can only displace the defender from the infinite defender cluster(s); the finite clusters are not invaded. One way to think of the process is to assign a random number r (chosen from a uniform distribution on [0,1]) to each site. When the occupation fraction is decreased from p to p-dp the invader displaces the defender from all sites which are in an infinite defender cluster and have random number r in the interval [p,p+dp].
- (2) The process ends when the defender percolation threshold is reached and the infinite defender cluster ceases to exist.

Since our purpose in this section is to compare percolation with trapping to ordinary percolation, we will first discuss ordinary percolation in an appropriate language. We again denote the two species as invader and defender and define p to be the occupation fraction of the defender. Initially the defender is at occupation fraction p = 1 and

forms a single infinite cluster. As p decreases, the defender will begin to break up into both finite clusters and one (or more) infinite cluster(s). For simplicity we will assume there is only one infinite cluster. If there is more than one, the term 'infinite cluster' will denote the union of the infinite clusters. We define P(p) to be the fraction of the defender occupied sites which are contained in the infinite cluster and $n_s(p)$ to be the number of finite clusters of size s (normalised per site). Then in ordinary percolation at any value of p we have the sum rule

$$\sum_{s=1}^{\infty} sn_s(p) + pP(p) + (1-p) = 1.$$
 (2.1)

The first term on the left represents the sites in finite defender clusters, the second those in the infinite defender cluster and the third in the sites occupied by the invader. Differentiating with respect to p we obtain

$$\sum_{s=1}^{\infty} s \frac{dn_s(p)}{dp} + p \frac{dP}{dp} = 1 - P(p).$$
 (2.2)

As we approach the defender percolation threshold at $p = p_c$, the quantities P(p) and $n_s(p)$ have the scaling behaviour (Stauffer 1979)

$$P(p) \sim \varepsilon^{\beta} \tag{2.3}$$

$$n_s(p) \sim s^{-\tau} f(s \varepsilon^{\Delta})$$
 (2.4)

where $\varepsilon = p - p_c$, f(x) is a scaling function and β , τ and Δ are universal critical exponents depending only on the dimension. A summary of percolation exponents and the relations between them is given in the appendix. Substituting into (2.2) we see that as $p \to p_c$ the terms on the left are divergent, while those on the right are finite. The requirement that the terms on the left cancel to leading order leads to the relation (Stauffer 1979)

$$\beta = \Delta(\tau - 2). \tag{2.5}$$

In percolation with trapping, the difference is that as we reduce the occupation fraction p, the defender is only depleted from the infinite cluster and not from the finite clusters. The infinite cluster is the same as it was in ordinary percolation but the finite clusters are different. The meaning of p is not now the fraction of sites occupied by the defender, but rather the fraction which would have been occupied by the defender if we had allowed the finite clusters to be depleted, i.e. it is a parameter which has the property that at a given value of p the infinite defender cluster is the same as it would have been in ordinary percolation. Let us denote the actual volume fraction of invader and defender at any particular value of p by $S_{\rm I}(p)$ and $S_{\rm D}(p)$. Because the invader can only enter the infinite defender cluster, when we decrease p infinitesimally from p to $p-{\rm d}p$ the invader fraction increases by an amount

$$dS_i = P(p) dp. (2.6)$$

Equation (2.6) is the fundamental equation in trapping percolation. Integrating we find

$$S_{I}(p) = \int_{p}^{1} P(p) dp.$$
 (2.7)

Let us denote by $\tilde{n}_s(p)$ the number of clusters of size s (normalised per site). Then we have

$$\sum_{s=1}^{\infty} s \tilde{n}_s(p) + p P(p) + \int_p^1 P(p) \, \mathrm{d}p = 1.$$
 (2.8)

As in (2.2), the first term represents the sites in finite defender clusters, the second the sites in the infinite defender cluster and the third the sites occupied by the invader. Differentiating with respect to p we obtain

$$\sum_{s=1}^{\infty} s \frac{\mathrm{d}\tilde{n}_s(p)}{\mathrm{d}p} + p \frac{\mathrm{d}P}{\mathrm{d}p} = 0. \tag{2.9}$$

Let us assume that as we approach the defender percolation threshold at $p = p_c$, the quantity $\tilde{n}_s(p)$ has the scaling behaviour

$$\tilde{n}_s(p) \sim s^{-\tilde{\tau}} \bar{f}(s \varepsilon^{\tilde{\Delta}})$$
 (2.10)

i.e. similar to (2.4), but possibly with different critical exponents and a different scaling function. Since the left-hand side of (2.9) is the same as that of (2.2), except for the appearance of \tilde{n}_s rather than n_s , when we substitute the critical behaviour in (2.9) we obtain a relation similar to (2.5):

$$\beta = \tilde{\Delta}(\tilde{\tau} - 2). \tag{2.11}$$

From (2.5) and (2.11) we see that if $\Delta = \tilde{\Delta}$ then it follows that $\tau = \tilde{\tau}$. We now argue heuristically that this should be the case. In ordinary percolation, the significance of the exponent Δ in (2.4) is that the typical size s_{max} of the largest clusters at a given value of p scales as

$$s_{\text{max}} \sim \varepsilon^{-\Delta}$$
. (2.12)

A similar interpretation holds for the exponent $\tilde{\Delta}$ in (2.10) for percolation with trapping. Both in ordinary percolation and in percolation with trapping, the largest finite defender clusters are generally those which have most recently been detached from the infinite cluster. It is thus reasonable to suppose that s_{max} should scale in the same way in both cases, since at the moment they are detached the finite clusters in percolation with trapping are the same as in ordinary percolation; only the subsequent development is different. Thus we conclude tentatively that the exponents in (2.4) and (2.10) are equal:

$$\tilde{\Delta} = \Delta$$
 $\tilde{\tau} = \tau$. (2.13)

As further evidence for (2.13), we have solved percolation with trapping exactly for the case of an infinite Cayley tree. For simplicity we consider the case of coordination number three, for which the percolation threshold is at $p_c = \frac{1}{2}$. In ordinary percolation at occupation fraction p, let us consider a site chosen at random together with two of the three branches connected to it. On these two branches, let Q(p) denote the probability that the site is in an infinite cluster and $Q_s(p)$ the probability that it is in a cluster of size s. The site itself is included in the count so that $Q_0(p) = 1 - p$ is the probability that the site is not occupied. It is easy to see that Q(p) satisfies

$$1 - Q = 1 - p + p(1 - Q)^{2}$$
(2.14)

and that if we define the generating function

$$\hat{Q}_{\alpha}(p) = \sum_{s=0}^{\infty} Q_{s}(p)\alpha^{s}$$
 (2.15)

then \hat{Q}_{α} satisfies

$$\hat{Q}_{\alpha} = 1 - p + \alpha p \hat{Q}_{\alpha}^{2}. \tag{2.16}$$

From these we may conclude that as $p \to \frac{1}{2}$

$$Q \sim \varepsilon$$
 (2.17)

$$Q_s \sim s^{-3/2} F(s\varepsilon^2) \tag{2.18}$$

where $\varepsilon = p - \frac{1}{2}$ and F(x) is a scaling function. By similar arguments it may be shown that the percolation exponents on the Cayley tree take the values (Fisher and Essam 1961)

$$\beta = 1 \qquad \Delta = 2 \qquad \tau = \frac{5}{2}. \tag{2.19}$$

In percolation with trapping, when we remove a defender occupied site at random, the number \tilde{n}_s of clusters of size s will increase if and only if one of the branches connected to it consists of s sites and the other two are not both finite (so that the chosen site was in an infinite cluster). Since there are three branches, we find

$$d\tilde{n}_s/dp = 3Q_s[1 - (1 - Q)^2]$$

$$= 3Q_sQ/p$$

$$\sim s^{-3/2}\varepsilon F(s\varepsilon^2)$$
(2.20)

where we have used (2.14), (2.17) and (2.18). But from the scaling hypothesis (2.10) we have

$$d\tilde{n}_s/dp \sim s^{1-\tau} \varepsilon^{\tilde{\Delta}-1} f'(s \varepsilon^{\tilde{\Delta}}). \tag{2.21}$$

Comparing (2.20) and (2.21) we obtain

$$\tilde{\Delta} = 2$$
 $\tilde{\tau} = \frac{5}{2}$

in agreement with the percolation values (2.19).

From here on we will drop the tildes on the exponents and investigate whether the relations (2.13) are consistent with Monte Carlo simulations of the process.

3. Monte Carlo simulation

In order to perform Monte Carlo simulations of percolation with trapping it is necessary to define the process for a finite system. We will adopt the following algorithm.

- (1) Consider a square lattice (in two dimensions) or simple cubic lattice (in three dimensions) of side L with periodic boundary conditions. Initially every site is occupied by the defender, which thus forms a single 'infinite' cluster.
- (2) At each time step the invader displaces the defender from a site chosen at random from the infinite defender cluster. A check is made to see if this has divided the infinite defender cluster into two or more disconnected parts. If it has, the largest part is retained as the new infinite cluster and the smaller part (or parts) identified as finite cluster(s). The latter subsequently remain unchanged.
- (3) When the new infinite cluster is smaller than or equal in size to a cluster which has previously been declared finite, the last move is taken back and the process stops. The previous infinite cluster is included in the list of finite clusters, and is thus always the biggest cluster.

Of course, the actual rules are to some extent arbitrary; in particular the way in which we decide that the defender percolation threshold has been reached. In order to check that the percolation threshold is indeed identified in a reasonable way, we first calculated from our simulations the value of the defender occupation fraction at which the process ended. From (2.6) it is easy to see that each time a site is removed from the infinite defender cluster, the defender occupation fraction p decreases by an amount

$$\delta p = p/N_{\infty} \tag{3.1}$$

where N_{∞} is the number of sites in the infinite defender cluster before the site is removed. Thus the value of p at step i+1 is related to that at step i by

$$p^{(i+1)} = p^{(i)} \frac{N_{\infty}^{(i)} - 1}{N_{\infty}^{(i)}}.$$
 (3.2)

If we denote the final value of p on a system of size L by p(L), then we should expect p(L) to have the scaling behaviour

$$p_c - p(L) \sim L^{-1/\nu}$$
 (3.3)

where p_c is the percolation threshold and ν is the correlation length exponent. This relation is plotted in figure 1. The values $\nu = 1.32$ and $\nu = 0.86$ obtained on the square and simple cubic lattices are in satisfactory agreement with the accepted values 1.33 and 0.88 in ordinary percolation.

We will be most interested in the number \tilde{n}_s of clusters of size s. In general this quantity is a function of both the occupation fraction p and the system size L. For simplicity we will concentrate on the final configuration, so that \tilde{n}_s is a function of L only. We will assume that $\tilde{n}_s(L)$ has the scaling form

$$\tilde{n}_s(L) \sim s^{-\tau} g(s/s_{\text{max}}) \tag{3.4}$$

where g(x) is a scaling function and s_{max} , which may be considered as the size of the largest cluster, scales as

$$s_{\max} \sim L^D. \tag{3.5}$$

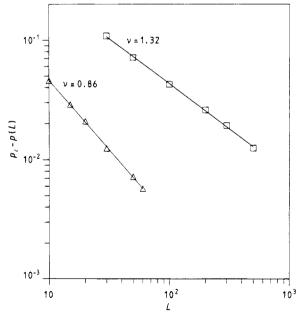


Figure 1. Plot of $p_c - p(L)$ against lattice size L for the square (\Box) and simple cubic (\triangle) lattice. The values of ν for the two plots are obtained by equating the slope to $1/\nu$ as in (3.3). The values of p_c used are $p_c = 0.5927$ on the square lattice (Derrida and de Seze 1982, Wilkinson and Barsony 1984) and $p_c = 0.3117$ on the cubic lattice (Heermann and Stauffer 1981, Wilkinson and Barsony 1984).

In accordance with the discussion of the previous section, we will tentatively identify τ and D as the cluster size exponent and fractal dimension of ordinary percolation. One natural way to attempt to extract the exponent τ is to plot the quantity

$$\tilde{N}_{s}(L) = \sum_{s'=s}^{2s-1} \tilde{n}_{s'}(L).$$
 (3.6)

For $1 \ll s \ll s_{max}$ this should scale as

$$\tilde{N}_{\rm s} \sim {\rm s}^{-(\tau-1)}.\tag{3.7}$$

The quantity (3.6) is plotted on a log-log plot as a function of s in figure 2. We see that there is an apparent straight portion and that the curves are 'humped', i.e. they rise above the extrapolated straight line before dropping off at large s. We will comment on this feature later. The estimates for τ obtained by fitting (3.7) for different lattice sizes are listed on the line labelled τ_N of table 1. We see that these estimates for τ show a tendency to increase with L and are considerably smaller than the accepted percolation values for τ of 2.05 in two dimensions and 2.21 in three dimensions. Furthermore the values in two dimensions are less than 2, which is impossible if

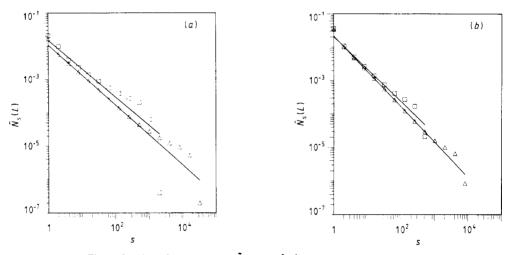


Figure 2. Plot of the quantity $\tilde{N}_s(L) = \sum_{s=s}^{2s-1} \tilde{n}_s(L)$ against s for different values of the lattice size L. (a) Square lattice, L = 100 (\square), 500 (\triangle); (b) cubic lattice, L = 20 (\square), 60 (\triangle). Observe that the curves rise above the extrapolated straight line before falling off at large s due to the finite lattice size. Values for the cluster size exponent τ obtained by fitting a straight line and using (3.7) are listed in table 1.

Table 1. Monte Carlo values of the cluster size exponent τ in percolation with trapping for different lattice sizes L. The values labelled τ_N were obtained by fitting (3.7) and those labelled τ_M by fitting (3.9). The values in ordinary percolation are $\tau = 2.05$ in 2D and $\tau = 2.21$ in 3D.

	2D				3D			
L	100	200	300	500	20	30	50	60
N	1.85	1.86	1.88	1.90	1.97	2.00	2.04	2.06
м	2.07	2.06	2.05	2.05	2.15	2.16	2.17	2.17

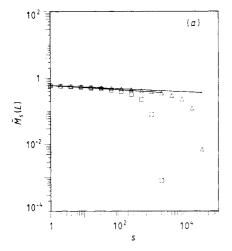
 $\sum_{s=1}^{\infty} s\tilde{n}_s$ is to converge. Since this result is also in contradiction with the theoretical arguments of the previous section, let us estimate the exponent τ in a different way by defining the quantity

$$\tilde{\mathbf{M}}_{s}(L) = \sum_{s'=s}^{\infty} s' \tilde{\mathbf{n}}_{s'}(L)$$
 (3.8)

which is the fraction of sites which are contained in clusters of size s and greater. From (3.4) this should scale for $1 \ll s \ll s_{\text{max}}$ as

$$\tilde{M}_s \sim s^{-(\tau-2)}. ag{3.9}$$

Since \tilde{M}_s is a decreasing function of s, it is clearly impossible that fitting (3.9) should lead to a value of τ less than 2. Indeed in figure 3 we see that the straight portion of the curve has negative slope, as expected. In addition the 'hump' in the curves is no longer present. The estimates for τ obtained by fitting (3.9) for different lattice sizes are shown on the line labelled τ_M of table 1. We see that the values obtained from the different lattice sizes are in better agreement with each other and are much closer to the values for ordinary percolation.



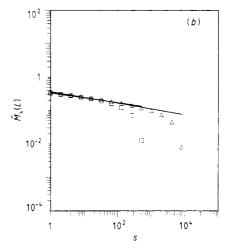


Figure 3. Plot of the quantity $M_s(L) = \sum_{s'=s}^{\infty} \tilde{n}_{s'}(L)$ against s for different values of the lattice size L. Values for the cluster size exponent τ obtained by fitting a straight line and using (3.9) are listed in table 1. ((a), (b) as in figure 2.)

The scaling function g(x) in (3.4) has an interesting property which, it turns out, explains why it is that the quantity \tilde{M}_s in (3.9) yields a better exponent estimate than \tilde{N}_s in (3.6). Let us consider the final value $S_D^*(L)$ of the defender saturation on a system of size L. From (2.7) we see that this is given by

$$S_{\rm D}^*(L) = 1 - \int_0^1 P_L(p) \, \mathrm{d}p$$
 (3.10)

where $P_L(p)$ is the fraction of defender occupied sites which are in the 'infinite' cluster on a system of size L at defender occupation fraction p. Thus (Wilkinson 1984)

$$S_{D}^{*}(\infty) - S_{D}^{*}(L) = \int_{0}^{1} (P_{L}(p) - P(p)) dp$$

$$\sim L^{-(1+\beta)/\nu}$$
(3.11)

since P(p) and $P_L(p)$ differ only over a region of extent $\varepsilon \sim L^{-1/\nu}$ around $p = p_c$. The quality of our Monte Carlo data is not good enough to obtain a good estimate of the exponent because $S_D^*(\infty)$ is not known. Therefore in figure 4 we have assumed that the exponent is correctly given by (3.11) and chosen $S_D^*(\infty)$ to give the best fit. Clearly the data are consistent with the relation (3.11).

In terms of $\tilde{n}_s(L)$, the quantity $S_D^*(L)$ is given by

$$S_{\mathrm{D}}^{*}(L) = \sum_{s=1}^{\infty} s \tilde{n}_{s}(L)$$
 (3.12)

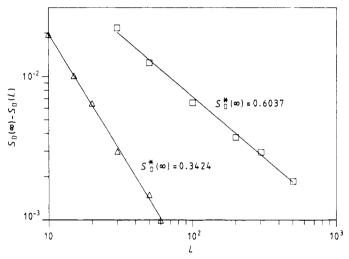


Figure 4. Plot of the quantity $S_D^*(\infty) - S_D^*(L)$ against lattice size L. In order to avoid attempting a three-parameter fit, the values for $S_D(\infty)$ indicated on the plots were obtained by requiring the slopes to agree with the prediction (3.11). Note that the values obtained for $S_D^*(\infty)$ are close to but larger than the percolation thresholds of 0.5927 for the square lattice and 0.3117 for the cubic lattice. This is due to the trapping rule which prevents disconnected clusters from being depleted. Lines, \square , square lattice; \triangle , cubic lattice.

so that

$$S_{\mathrm{D}}^{*}(L) - S_{\mathrm{D}}^{*}(\infty) = \sum_{s=1}^{\infty} s(\tilde{n}_{s}(L) - \tilde{n}_{s}(\infty))$$

$$\sim s_{\max}^{2-\tau} \int_{0}^{\infty} x^{1-\tau} \hat{g}(x) \, \mathrm{d}x$$
(3.13)

where

$$\hat{g}(x) = g(x) - g(0). \tag{3.14}$$

Using (3.13) and the exponent relations listed in the appendix we obtain

$$S_{\rm D}^*(L) - S_{\rm D}^*(\infty) \sim L^{-\beta/\nu} \int_0^\infty x^{1-\tau} \hat{g}(x) \, \mathrm{d}x.$$
 (3.15)

Comparing (3.15) and (3.11) we find that g(x) must satisfy the integral identity

$$\int_0^\infty x^{1-\tau} \hat{g}(x) \, \mathrm{d}x = 0. \tag{3.16}$$

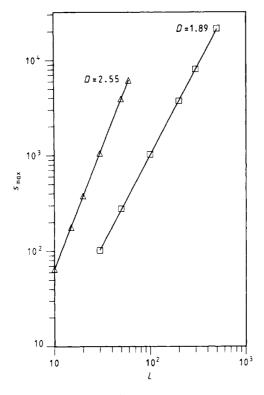


Figure 5. Plot of the size S_{\max} of the largest cluster for against lattice size L. According to (3.5) the slope D should be the fractal dimension of ordinary percolation. Lines, \square , square lattice; \triangle , cubic lattice.

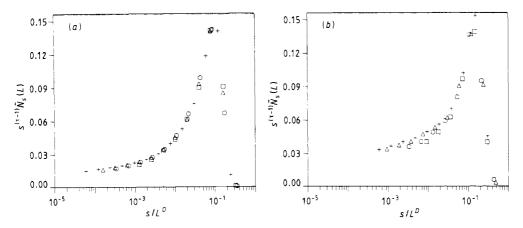


Figure 6. Plot of the quantity $s^{r-1}\tilde{N}_s(L)$ against the scaling variable s/L^D for different lattice sizes L. The exponent values used are given in table 2. The points plotted correspond to $s \ge 4$ for the square lattice and $s \ge 5$ for the cubic lattice. (a) Square lattice, L = 100 (\square), 200 (\square), 300 (\triangle), 500 (+); (b) cubic lattice, L = 20 (\square), 30 (\square), 50 (\triangle), 60 (+).

This explains the 'hump' in the curves of figure 2. At large x the function g(x) goes to zero and $\hat{g}(x)$ is negative. Thus at small x the quantity $\hat{g}(x)$ must be positive and a log-log plot of \tilde{n}_s or \tilde{N}_s against s must rise above the extrapolated straight line before dropping off at large s. The relation (3.16) also explains why \tilde{M}_s is less sensitive to finite-size correlations than \tilde{N}_s :

$$\tilde{M}_{s}(L) = \sum_{s}^{\infty} s\tilde{n}_{s}(L)$$

$$= \sum_{s}^{\infty} s\tilde{n}_{s}(\infty) + \sum_{s}^{\infty} s(\tilde{n}_{s}(L) - \tilde{n}_{s}(\infty))$$

$$\sim \frac{g(0)}{\tau - 2} s^{2 - \tau} + s_{\text{max}}^{2 - \tau} \int_{x}^{\infty} x^{1 - \tau} \hat{g}(x) dx$$

$$\sim \frac{g(0)}{\tau - 2} s^{2 - \tau} - s_{\text{max}}^{2 - \tau} \int_{0}^{x} x^{1 - \tau} \hat{g}(x) dx$$

$$= \frac{g(0)}{\tau - 2} s^{-(\tau - 2)} \left(1 - \frac{\tau - 2}{g(0)} x^{\tau - 2} \int_{0}^{x} x^{1 - \tau} \hat{g}(x) dx \right) \tag{3.17}$$

where $x=s/s_{\rm max}$ and we have used (3.16) in going from line three to line four. If we make the simplest hypothesis, that $\hat{g}(x)$ is positive for small x and negative for large x with only one zero in between, then the contribution of the second term in the large bracket, which represents the leading correction to the power law (3.9), is always negative. This explains why the curves in figure 3 deviate monotonically from straight lines—there is no hump as in figure 2. Furthermore the factor $\tau-2$ multiplying the correction term suggests that the finite-size scaling effects will be small for $\tilde{M}_s(L)$, because τ is close to two. The erroneous results obtained with the quantity \tilde{N}_s are due partly to the larger finite-size effects and partly to the 'hump' in the curve which leads to a straight line fit with too small a slope. We conclude that the Monte Carlo results are consistent with the hypothesis that the exponent τ is the same as in ordinary percolation.

In going from (3.14) to (3.15) we have implicitly assumed that the exponent D is (3.5) is the same as the fractal dimension of ordinary percolation. In order to check this directly, in figure 5 we have plotted the average size of the largest cluster as a function of the lattice size L. The values D=1.89 and D=2.55 are in reasonable agreement with the values 1.90 and 2.49 of ordinary percolation. Finally in order to check the scaling form (3.4) itself, we observe that the quantity $s^{\tau-1}\tilde{N}_s$ should be a function only of the scaling variable $x=s/L^D$, and not of s and L separately. In figure 6 we have plotted this relationship, assuming the percolation values for τ and D. The fact that the points for different L fall on a single curve suggests strongly that the scaling hypothesis (3.4) is correct, and that the critical exponents are the same as those of ordinary percolation.

4. Discussion

The purpose of this paper has been to introduce a new form of percolation which we call 'percolation with trapping' and to suggest that its critical behaviour may be

understood in terms of the critical exponents of ordinary percolation. Although we have not been able to prove this rigorously, we believe that the theoretical arguments of § 2 and the Monte Carlo results of § 3 provide compelling evidence for the correctness of this hypothesis. A critical reader might suggest that the quality of the Monte Carlo data is not really sufficient to come to this conclusion; in particular the system sizes used ($L_{\rm max} = 500$ in two dimensions and $L_{\rm max} = 60$ in three dimensions) are not as large as the best Monte Carlo work in ordinary percolation. This is inevitable, since percolation with trapping is much more difficult to simulate than ordinary percolation, because of the necessity of checking at each step whether the 'infinite' cluster has been broken. However, we would claim that the Monte Carlo data show no evidence that percolation with trapping is in a different universality class from ordinary percolation.

Percolation with trapping is an interesting process which sheds light on the way in which the infinite percolation cluster is broken up as the occupation fraction is decreased. It also provides a natural way, free of boundary effects, of identifying the percolation threshold on a finite system (see the discussion at the beginning of § 3). In considering how this definition might be used in ordinary percolation, we have realised that there exists a different, more efficient, way of simulating percolation with trapping which emphasises even more strongly its connection with ordinary percolation. The key observation is that in percolation with trapping we can, if we wish, allow the finite defender clusters to be invaded (provided we keep track of the sizes of the clusters when they are first detached from the infinite cluster), because the way in which the infinite defender cluster is broken up is independent of what happens to the finite defender clusters. Since, then, the process is precisely the same as ordinary percolation (above threshold), this suggests that it should be possible to obtain the same information by performing the simulation in reverse, i.e. start at 'defender' occupation fraction p=0 rather than at p=1. Consider the following algorithm on a lattice of side L with periodic boundary conditions.

- (1) Start at occupation fraction p=0 and gradually increase p by adding one randomly chosen site at a time (just as in ordinary percolation). Each time a site is added, it either forms an isolated one-site cluster, or joins a previously existing cluster, or connects together two or more previously existing clusters. In the latter case, if the new cluster becomes (strictly) the largest cluster, then record the sizes of the clusters from which it was formed, omitting any cluster equal in size to the previous largest cluster. Record also the size of the largest cluster after each step.
 - (2) Continue the process until the entire lattice is filled.
- (3) At the end we have (for each step) a list of clusters (if any) added to the new largest cluster and the size of the new largest cluster itself. Thus we know the size of the largest added cluster (counting all the steps). Let us identify the percolation threshold $p_c(L)$ for the given realisation as the occupation fraction at which the largest cluster first becomes (strictly) larger than this largest added cluster. By comparing this algorithm to our direct simulation of percolation with trapping (with the sites removed in the opposite order), it is easy to convince oneself that the percolation threshold is defined in the same way, and that above the percolation threshold the added clusters in the new method are precisely those identified as finite clusters in percolation with trapping.

At first sight it might appear that the new algorithm is both more complicated and more costly, because we have to simulate the entire process from p = 0 to p = 1 rather than just the portion above p_c . However, in practice it is much more efficient, because keeping track of the connectedness as p increases is much simpler than deciding when

the 'infinite' cluster has been broken as p decreases. Although we have not investigated this idea in detail, preliminary estimates suggest that the above algorithm is indeed superior in both speed and storage requirements to the algorithm employed in \S 3.

The physical significance of this paper is that the incompressibility of the displaced phase in immiscible displacement in porous media does not prevent the critical behaviour from being understood in terms of ordinary percolation exponents. A critical reader might object that percolation with trapping is an over-simplified version of the full displacement model (invasion percolation with trapping), since it does not take account of the requirement that the displacing phase form a connected cluster. Let us address this objection in two ways.

Firstly, it is possible to envisage a situation where percolation with trapping is a qualitatively correct model of the fluid displacement process, i.e. when the displacing phase is perfectly wetting. If the flow rate is low enough then the wetting phase can first reach all parts of the sample by transport in wetting films and roughness of the pore walls, without bulk occupation of any of the pores or throats. As the capillary pressure is decreased, these surface films grow and can become unstable, resulting in a 'snap-off event in which the non-wetting fluid is suddenly displaced from a throat. This leads to a bond (rather than site) version of percolation with trapping, since the throats which become occupied by the wetting fluid need not form a connected set. Since one would expect the bond and site problems to have the same critical behaviour, percolation with trapping may thus be a good qualitative model of the displacement process in this case.

A second reason for studying percolation with trapping is that, even though it is a different process from invasion percolation with trapping, it can possibly yield the same critical behaviour at the defender percolation threshold (at least in three dimensions). The key feature of invasion percolation with trapping is that the trapping of the defender takes place in the presence of only a single invader cluster, rather than many invader clusters as in percolation with trapping. For two-dimensional planar lattices this distinction is very important, since in invasion percolation with trapping the two percolation thresholds necessarily occur together, while in percolation with trapping the defender becomes disconnected (and the process stops) before the invader percolates (this is related to the fact that $p_c > \frac{1}{2}$). Indeed, as observed in the introduction, there is Monte Carlo evidence to suggest that invasion percolation with trapping in two dimensions is in a different universality class from ordinary percolation. In three dimensions, however, the situation is different. Both in invasion percolation with trapping and percolation with trapping (and in ordinary percolation) the invader percolates long before the defender becomes disconnected. At the defender percolation threshold the invader is well above threshold and so in percolation with trapping most of the invader is in a single large cluster. Thus it is perhaps reasonable to suppose that the critical behaviours for percolation with trapping and invasion percolation with trapping are the same in three dimensions. This idea has been used successfully (Wilkinson 1984) in computer simulations of the effects of buoyancy (density difference) on the displacement process. On the other hand, it is in disagreement with other direct Monte Carlo data on invasion percolation with trapping (Wilkinson and Willemsen 1983, Willemsen 1984) which suggests that, even in three dimensions, the scaling properties of the defender cluster size distribution are different from those of ordinary percolation. Although the present work does not directly address this question, we believe that these earlier papers (which suggested a value $\tilde{\tau} \sim 2.05$ -2.07 in three dimensions) may be in error because the value of $\tilde{\tau}$ was estimated from the quantity analogous to our \tilde{N}_s in (3.6). As we have seen, use of this quantity can lead to too low a value for $\tilde{\tau}$.

In summary, we have investigated a modified version of percolation, 'percolation with trapping', which is motivated by the fluid-fluid displacement in porous media and have concluded that its critical behaviour may be understood in terms of ordinary percolation exponents.

Appendix

In this appendix we list the definitions of the critical exponents of ordinary percolation, the relations between them and their generally accepted values in two and three dimensions. We denote the occupation fraction by p and the critical percolation threshold by p_c . In the applications of this paper we are always above threshold, so $\varepsilon = p - p_c$ is positive. We define P(p) to be the fraction of occupied sites which are in the infinite cluster and $n_s(p)$ to be the number of finite clusters of size s (normalised per site). As $\varepsilon = p - p_c \rightarrow 0$ these have the behaviours (Stauffer 1979)

$$P(p) \sim \varepsilon^{\beta}$$
 (A1)

$$n_s(p) \sim s^{-\tau} f(s \varepsilon^{\Delta})$$
 (A2)

where f(x) is a scaling function and β , Δ and τ are the magnetic, gap and cluster size exponents respectively. As shown in § 2, these satisfy the scaling relation

$$\beta = \Delta(\tau - 2). \tag{A3}$$

The correlation length ξ , which is the typical size of the largest finite clusters, scales as

$$\xi \sim \varepsilon^{-\nu}$$
 (A4)

where ν is the correlation length exponent, which is related to the other exponents and the space dimension d via the hyperscaling relationship

$$d\nu = \beta + \Delta. \tag{A5}$$

At threshold the infinite cluster is a fractal with fractal dimension D, which is related to the other exponents by

$$D = d - \beta / \nu = \Delta / \nu. \tag{A6}$$

Values of the critical exponents in two and three dimensions are listed in table 2.

Table 2. Accepted values of the various percolation exponents in two and three dimensions. The values in 2D are exact (den Nijs 1979). The values in 3D are computed from relations (A3)-(A6) and the values $\beta = 0.45$ and $\nu = 0.88$ (Heermann and Stauffer 1981, Gaunt and Sykes 1983, Wilkinson and Barsony 1984).

	2D	3D		
β	5/36	0.45		
ν	4/3	0.88		
Δ	91/36	2.19		
au	187/91	2.21		
D	91/48	2.49		

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