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Percolation and invasion percolation in the presence of mobile impurities

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Abstract. We present a model for the solidification process of two immiscible fluids interacting repulsively with mobile impurities on a two-dimensional square lattice. In the space of the fluids and impurity concentrations, the phase diagram exhibits a critical curve separating a percolating from a non-percolating phase. Estimated values for the fractal dimension and the exponent β of the order parameter reveal that the critical exponents do not vary along this curve, i.e., they are independent of the impurity concentration. The universality class is that of the ordinary percolation. On the basis of the ideas of the dynamic epidemic and invasion percolation models, we also propose a model that may be relevant to cleaning porous media by fluid injection. An analysis of the acceptance profile, the fractal dimension and the gap exponent strongly indicate that this model belongs to the universality class of the ordinary invasion percolation.

1. Introduction

The percolation theory has a fundamental role in the study of many interesting phenomena occurring in nature [1, 2]. It has been successfully applied to a variety of systems, including conductivity problems, kinetic gelation, magnetic disordered systems and fluid flow in porous media [3].

Although originally formulated as a static problem, the percolation concept has also prospered in dynamical systems. Among several dynamic growth models which deal with percolating clusters, the epidemic models are particularly significant [4, 5].

Recently, a simple theoretical model, namely the dynamic epidemic model [6, 7], has been proposed to describe the growth of a solid interface through a liquid in the presence of impurity particles. A repulsive interaction exists between the solid phase and the particles. The advancing front obeys the Eden model growth rules [8]. The solid front pushes away the impurities and may lead to the formation of aggregates which are hindrances to the growth. Depending on the concentration x_I of the impurities, a phase transition may occur separating a finite from an infinite spreading out of the solid phase.

The idea of the repulsive solid–particle interaction came from the so-called UCJ mechanism (Uhlmann, Chalmers and Jackson [9]). They found this short-range interaction in experiments in which a solid front advances through a liquid in the presence of mobile impurities. Moreover, depending on the solidifying velocity there is a critical value below which the impurity particles are indefinitely pushed ahead into the liquid, travelling along the interface. Above this critical value the impurities are trapped in the solid phase.

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The dynamic epidemic model was numerically studied in both two and three dimensions [6,7]. It exhibits a blocking transition at the values $x_I = 0.56$ and 0.80 for the square and simple cubic lattices, respectively. These values are quite different from those for the static epidemic model (i.e., the ordinary site percolation model) which are 0.41 and 0.69 (the complements of the critical thresholds).

In section 2 we extend the dynamic epidemic model to treat the solidification process of two immiscible fluids A and B in the presence of mobile impurities. We get the phase diagram in the concentration space by determining the order parameter. A line of critical points is found. A careful analysis of the cluster fractal dimensions as well as of the exponent β of the order parameter does not show any dependence on the concentrations, implying that universality holds along the critical line. In section 3, we study a different model. It is intended to describe a process of cleaning a dirty porous medium. The fractal dimensions and the gap exponent are estimated. They suggest that this system is in the same universality class as the invasion percolation model.

2. The dynamic percolation model

The lattice model can be defined as follows. First, a fraction x_I of the lattice sites are randomly occupied by impurities. The remaining sites are occupied either by a fluid of kind A with concentration x_A or by a fluid of kind B with concentration x_B. Of course, the constraint $x_I + x_A + x_B = 1$ always holds. We will assume that these two fluids are immiscible and that the system is in contact with a thermal reservoir kept at the (higher) solidification temperature of the fluid A.

The growth process starts by putting, at the lattice centre, a solid unit of kind A. At each time step, a *liquid* site of kind A which is in contact with the solid front is randomly chosen and turned to *solid*. If liquid sites of kind A are no longer available the solidification process stops. Let us now describe how the UCJ mechanism of repulsive short-range interactions between the solid front and mobile impurities is simply introduced in our simulations. When an impurity is touched by a newly added *solid* unit, it moves toward a randomly chosen nearest neighbour (exchanging places with a *liquid* site A or B) if this action reduces its number of contacts with the solid front. Otherwise, the impurity remains in the same place.

Besides pushing the impurities, our model has also characteristics peculiar to percolation problems: the cluster of the solid phase A may span the whole lattice or not. Thus we expect a critical curve in the plane $x_I + x_A + x_B = 1$ of the concentration space. Without impurities ($x_I = 0$), our model reduces to the well known Leath model [4] where fluids of kind A (B) correspond to the occupied (blocked) sites. Another particular case arises for $x_B = 0$ when the standard dynamic epidemic model [6] is recovered.

Numerical simulations were carried out on square lattices of size $L = 201, 401, 801$ and 1601. For each value of x_I, we performed a number of experiments sufficient to reduce the statistical error to less than one per cent. The phase diagram was obtained by determining the spanning probability, which is the probability that a lattice of linear dimension L percolates at concentration x_A [1]. We say that a system percolates if at least one cluster connects two opposite frontiers of the lattice. Figure 1 shows the x_A-dependence of the spanning probability for $x_I = 0.45$ and several lattice sizes. In the thermodynamic limit, a well marked phase transition occurs at some x_A^c, i.e., a critical threshold exists setting a continuous phase transition between two regimes: the percolating and non-percolating phases.

Figure 2 shows the phase diagram in the concentration space. As expected, if $x_I = 0$ the ordinary (site) percolation model is obtained. On the other hand, at $x_B = 0$, the growth mechanism is that of the Eden model and the standard dynamic epidemic model is recovered.

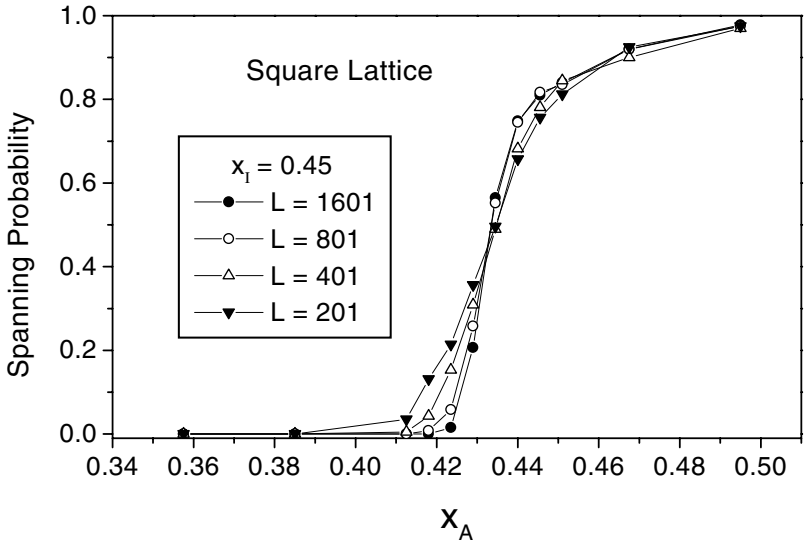

Figure 1. The spanning probability as a function of the fluid concentration x_A for $x_I = 0.45$ and several square-lattice sizes. A phase transition occurs at some x_A^c.

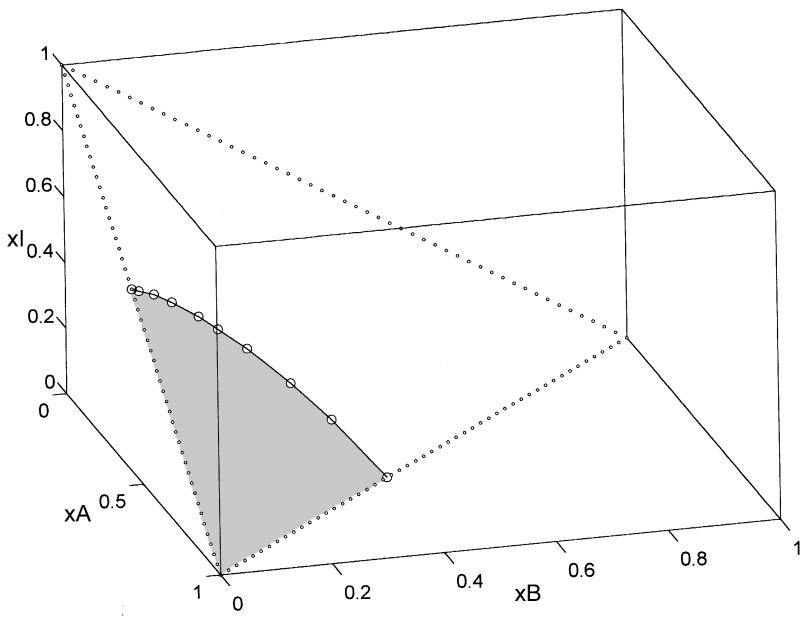

Figure 2. The phase diagram in the concentration space x_I, x_A, x_B. Only paths on the plane $x_I + x_A + x_B = 1$ are thermodynamically allowed. A critical line separates a percolating (grey area) from a non-percolating phase.

In general, there is a critical curve separating a finite from an infinite (represented by the grey area in the figure 2) growth phases.

A simple way to characterize the critical clusters is by evaluating their fractal dimensions [2, 10]. To do this, we investigate how the average mass $\langle M \rangle$ of the critical percolating clusters

scales with the mean gyration radius $\langle R_g \rangle$. The good quality of our data can be seen in figure 3. The error bars are smaller than the symbols used for the central values. Along the critical line we found that the values of the fractal dimensions are unique and equal to 1.89—that is, equal to the critical ordinary percolation value. Inside the percolating region the fractal dimension like in the Eden model is equal to 2.

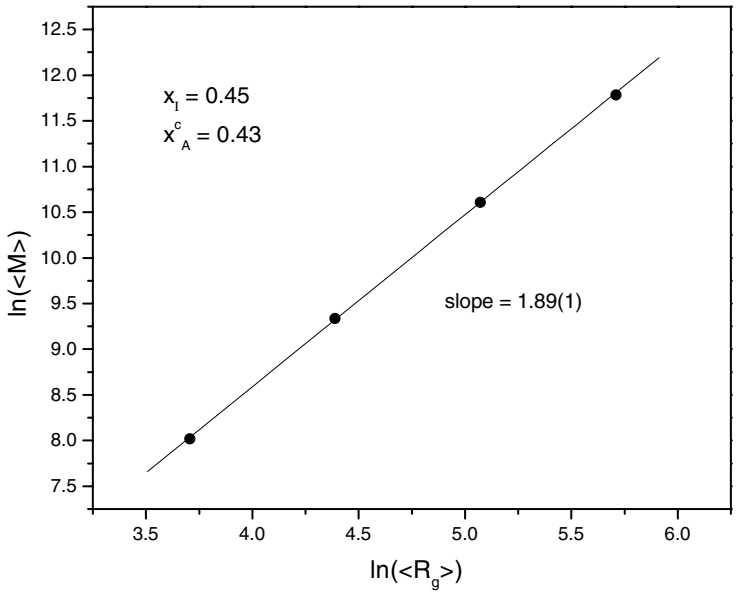

Figure 3. A log–log plot of the average mass versus the mean gyration radius. The slope of the straight line is the fractal dimension.

As is well known [1], the average density $\rho = \langle M \rangle / L^2$ is equal to the strength of the order parameter. This means that near the critical point we have $\rho \sim L^{-\beta/\nu} \sim ||x_A - x_A^c||^\beta$. By carrying out simulations very close to this point, we can estimate the critical exponent β. We have done such a calculation for several concentrations x_I and found always the same value $\beta \approx 0.15$ (see figure 4) which is compatible with the exact value $5/36$ for the ordinary percolation. Together with our results for the fractal dimension, this leads us to conclude that our model belongs to the ordinary percolation class of universality. Some typical clusters of the model are shown in figure 5.

3. The dynamic invasion percolation model

Invasion percolation [11] is a theoretical model used to describe fluid–fluid displacements in porous media. It is a kind of self-organizing criticality [12–14] exhibiting a scale-invariant behaviour in both space and time.

In computer simulations of the ordinary invasion percolation, we assign a random number r, uniformly distributed in the range [0, 1], to each lattice site and choose the central site as the seed of the growth. The perimeter sites of the cluster are identified as the growth sites. At each growth step, only one site of the perimeter is occupied—that with the smallest associated random number. The growth process is interrupted after the cluster reaches the lattice boundary.

Here, we implement an invasion percolation model in a porous medium such that a fraction x_I of the pores are occupied by mobile particles of dirty material (impurities). The

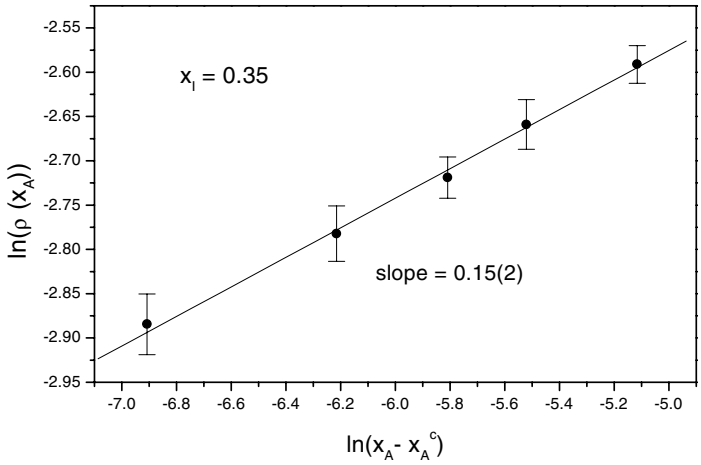

Figure 4. A log–log plot of the average density ρ (averaged out over 1000 instances) against $||x_A - x_A^c||$. The error bars are statistical deviations.

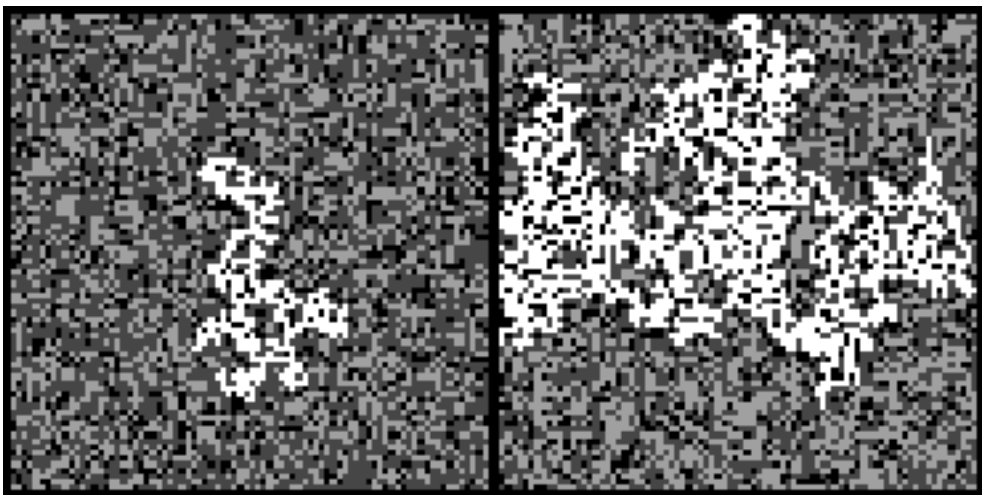

Figure 5. Some typical clusters of the dynamic percolation model at the mobile impurity concentration $x_I = 0.15$. The black (white) points represent the mobile impurities (solid A) and dark (light) grey the fluid B (A), respectively. The left (right) figures correspond to runs below (near) the critical threshold $x_A^c = 0.61$ in an 80×80 square lattice.

remaining pores have associated a random number r (also coming from a uniform distribution) corresponding to the pore's size. A fluid is injected at the centre of the lattice. From its first-neighbour empty pores, that with the smallest pore size is chosen to be invaded. This theoretical procedure mimics what really happens on an experimental level when the fluid flux is very low. Thus, viscous forces are irrelevant and the flow is dominated by capillary forces. We will assume that when the fluid touches an impurity a repulsive interaction of the UCJ kind appears. So, particles of dirty material will be pushed to fill empty pores.

We found a critical value of x_I^c above which the invading cluster is completely blocked. This value coincides with that obtained by Ausloos and Vandewalle [6] for the dynamic

epidemic model ($x_{\mathrm{I}}^c \simeq 0.56$ for the square lattice). For $x_{\mathrm{I}} < x_{\mathrm{I}}^c$ the fractal dimensions of the invading clusters are all equal and coincident with that of the ordinary invasion percolation. No dependence on x_{I} was found.

The acceptance profile $a(r)$ is a very useful concept introduced by Wilkinson and Willemsen [11] to study ordinary invasion percolation. They defined $a(r)$ as the ratio between the number of random numbers in the interval $[r, r + \mathrm{d}r]$ which were accepted into the cluster and the number of random numbers in that range which became available. In the limit of an infinite lattice, the acceptance profile tends to a step function with the discontinuity point r_c equal to the critical ordinary percolation threshold p_c.

Acceptance profiles can also be calculated in the dynamic invasion percolation model. In figure 6 we give the dependence of r_c on the impurity concentration x_{I}. For fixed values of x_{I} there is no tuning parameter, but even so the system is critical, indicating that it belongs to the class of self-organized criticality models.

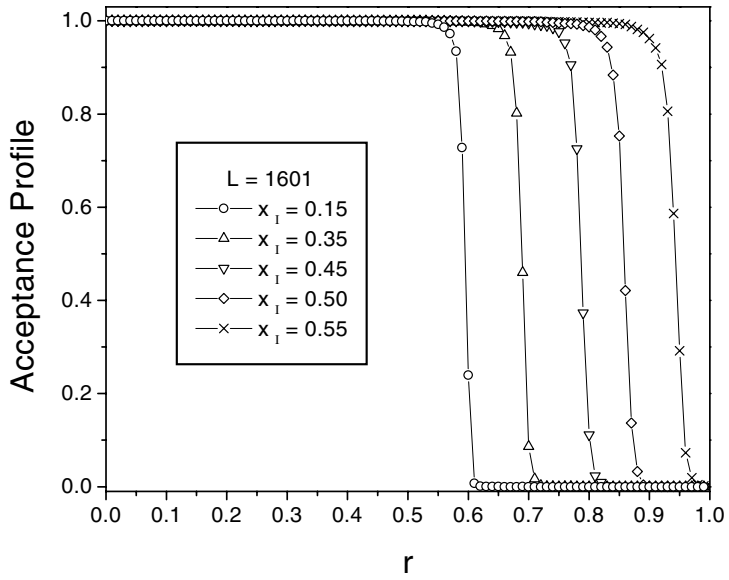

Figure 6. The acceptance profile behaviour for different values of x_{I}. The values of r_c increase with x_{I} up to $r_c = 1$, at which point $x_{\mathrm{I}} = 0.56$.

The acceptance profiles can be used to obtain the gap exponent $\Delta = \gamma + \beta$. Following Wilkinson and Barsony [15], we define the quantities

$$B_1 = \int_0^{r_c} (1 - a(r))\, \mathrm{d}r \tag{1}$$

and

$$B_2 = \int_{r_c}^{1} a(r)\, \mathrm{d}r \tag{2}$$

which represent the deviation of $a(r)$ from the step function. Applying finite-size arguments it can be shown that

$$B_1 = B_2 \approx \langle M \rangle^{-1/\Delta} \tag{3}$$

where $\langle M \rangle$ is the mean cluster mass. The logarithm plot is shown in figure 7 for impurity concentration $x_{\mathrm{I}} = 0.41$.

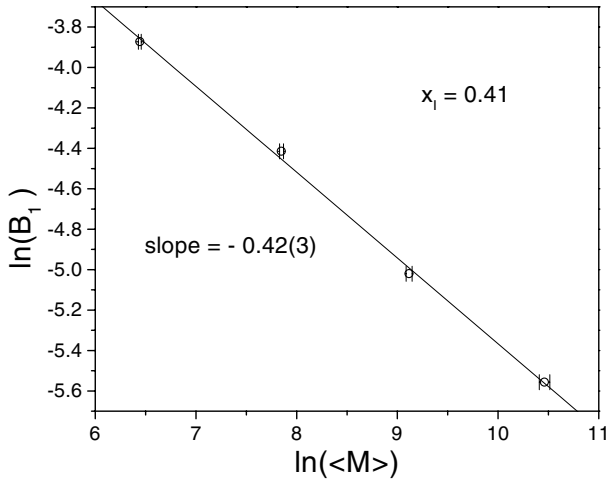

Figure 7. The slope of the curve is associated with the gap exponent. The points shown correspond to lattice sizes 101, 201, 401 and 801.

For $x_{\mathrm{I}} = 0.20, 0.35, 0.41$ we found $1/\Delta \simeq 0.43(3)$, $1/\Delta \simeq 0.41(3)$, $1/\Delta \simeq 0.42(3)$, respectively. These values are in reasonable agreement with the exact value for the ordinary percolation model ($1/\Delta = 36/91 \simeq 0.40$). Some typical clusters of the model are shown in figure 8.

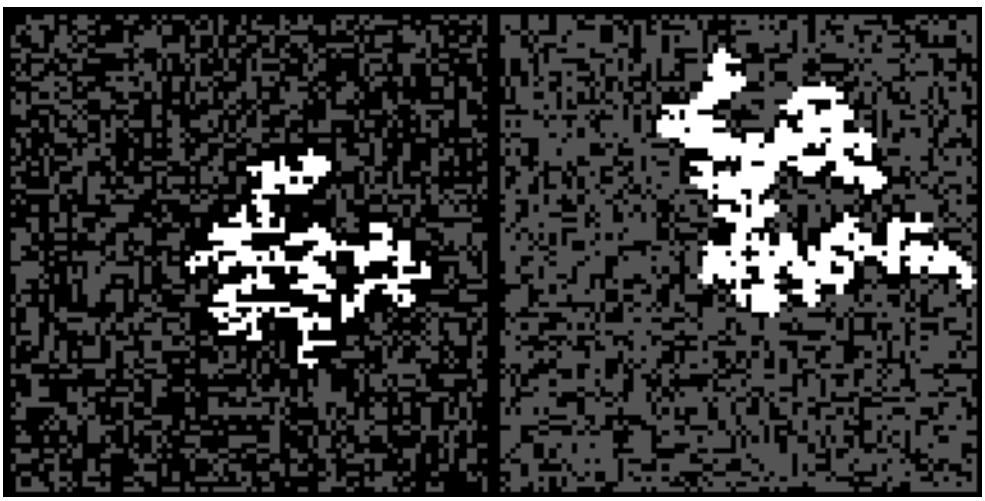

Figure 8. Some typical clusters of the dynamic invasion percolation model simulated at concentrations below (left) and above (right) the critical threshold $x_{\mathrm{I}}^{c} = 0.56$. The black and white points correspond to the impurities and the invader fluid, respectively.

4. Discussion

We present a dynamic percolation model and a dynamic invasion percolation model. The first is a solidification model of two immiscible fluids A and B in the presence of impurities

and in contact with a thermal reservoir at the melting point of fluid A. The phase diagram in the concentration space exhibits a critical percolation curve separating a percolating phase from a non-percolating phase. Our results firmly indicate that the critical exponents do not vary along this curve and, moreover, that the universality class is simply that of the critical ordinary percolation. In future works, it would be interesting to introduce a real temperature parameter (through energy interactions between fluids A and B and the impurity) in order to study the system behaviour when the (smaller) solidification temperature of the second fluid B is approached. If the solid A does not percolate and if the concentration x_I of impurities is not too high, then a new percolation phase transition can exist (but now at the solidification point of the fluid B). Certainly, for a given system (i.e., for fixed concentrations of impurities and of fluids A and B) these two percolation phase transitions are mutually exclusive. Note that this second transition would occur under a quite different condition: fluid B is in contact with immobile clusters (or isolated sites) of solid A and with partially mobile impurities (since now they can jump only to sites filled by the unfrozen fluid B).

The second model corresponds to a process of injecting fluid in a dirty porous medium. Smaller pores are occupied first and dirty particles are pushed away. An analysis of the fractal dimensions and acceptance profiles as well as of the gap exponent strongly suggested that this model is indeed a critical case. Were the repulsive interaction between the fluid and the dirty material a little stronger (to push not only a few particles but a whole cluster of dirty particles), then certainly this model would be a good candidate for describing a process of cleaning a dirty porous medium. Further studies of the model may, for example, introduce a new dynamics with successive cycles (as has been done recently for the dynamic epidemic model [16]). Such an investigation might be relevant to explaining how salt is left behind by water flowing in a porous system like cement.

Acknowledgments

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