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Microscopic-Based Fluid Flow Invasion Simulations

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A microscopic method for the generation of invasion percolation structures using "armies" of interacting random walkers is presented. Two distinct species are used to simulate the invading and defending fluids of a fluid invasion process. Trapping of the defending species is accomplished purely by local rules, without the need to repetitively check the connection between the "to be displaced" defender phase and the sink.

KEY WORDS: Porous media; simulation; random walkers; trapping.

1. INTRODUCTION

Problems concerning flow through porous media permeate many disciplines, from living systems (blood flow) to ancient rocks (oil recovery[1]). Percolation theory[2] recognizes the network aspect of flow in porous media, but provides only a very limited characterization of the fluid.[3-6] In particular, percolation theory contains no dynamics; indeed, it applies only to infinitely slow processes. Koplik and Lasseter[7] attempted to treat the dynamics of the flow by solving the appropriate differential equations of a very small network, but were limited due to computability. Lenormand and Zarcone[8,9] retained the lattice formulation typical of the percolation method, but developed a "local" approach to the trapping of defender clusters, utilizing the Kirkpatrick relaxation method.[10] Their approach was to define a pressure at every node, then update these pressures, and the invader front advance, each time step. By not allowing complete relaxation between time steps, they incorporated the dynamic behavior in a very elegant fashion.

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Of interest in flow in porous media are two fundamental and related phenomena, fingering and trapping. Fingering is a result of perturbations at the interface which are enhanced as the invasion takes place.[11,12] The result is a "sweep" of the medium where fingers of invader fluid, separated by regions of defender fluid, propagate through the medium. Trapping occurs when portions of the defender phase become surrounded by the invading phase and the invading phase cuts off the last remaining connection of the defender cluster to the sink. In the absence of any compressibility of the defender, this cluster represents a region of the network that is inaccessible to the invading phase. The complexity of these phenomena lies in the nonlocal nature of the problem.[3]

In this paper we implement recent methods of simulating fluid flow[14],[2] and chemical reaction kinetics[15] involving the use of discrete entities, specifically systems of random walkers, in order to generate invasion structures dynamically. A set of microscopic rules can be incorporated with these techniques to simulate a variety of nonlinear behavior while maintaining the simplicity of the rules. Most importantly, the rules are entirely local, even for the trapping, making the test of connectivity to a sink unnecessary. The result is a complex structure of invader fluid patterns which exhibits defender fluid trapping. We find, for unequal viscosities, that the patterns span those expected for viscous fingering to those for a very dense and efficient sweep.

In our extension of the simulation method, a second species of walkers is introduced,[16] one species to represent each of the two fluid phases, with an additional rule governing interfacial interactions which results in the trapping of defender fluid clusters as well as the fingering phenomenon. One interpretation of this additional rule is a constraint on the walk of the defender walkers that they may not walk where an invader walker has been. This simple asymmetry is all that is required to generate fingering and trap defender fluid clusters!

2. THEORETICAL CONSIDERATIONS

We presume that transients in pressure decay according to a diffusion equation so that in our case the two fluids are governed by a set of time-dependent diffusion equations coupled at the interfacial boundary. Since we wish to model diffusion on a grid, we write the diffusion equation in finite

[2] A related and rather elegant approach developed by King and Scher,[13] which is equivalent to a random walk under specific conditions, stochastically evolves saturation contour lines that also incorporates trapping via local rules.

difference form and obtain the following result for the transient of the invader pressure P_i:

$$P_i(x, y, t+\Delta t) = \left(1 - \frac{D_i \Delta t}{\Delta x^2}\right) P_i(x, y, t) + \frac{D_i \Delta t}{4\Delta x^2} [P_i(x+\Delta x, y, t) + P_i(x-\Delta x, y, t) + P_i(x, y+\Delta y, t) + P_i(x, y-\Delta y, t)]$$

with a similar equation for the defender pressure P_d. If $\Delta x = \Delta y$ and $D_i = \Delta x^2/\Delta t$, the first term on the rhs in this equation disappears and one obtains the equation governing the usual random walk, where the P_i now represents "occupancy probabilities" of the site (x, y) at time t. The diffusivities are inversely proportional to the viscosities, so that we can vary the viscosity ratio by a change in the ratio of diffusivities. Although it is clear that the form of the equation for the diffusion of pressure can be emulated by a random walk, the coupling of the pressure "fields" at the interface is by no means trivial.

For the moment let us imagine that, in the random walker formulation of the problem, the interface between the two phases has just evolved to a new location and, as a result, the pressures within the distinct phases are not the steady-state pressures. At this instant one would expect that the invader pressures near the interface are too low, and the defender pressures near the interface are too high. Hence, the subsequent bulk relaxation processes will involve additional invader walkers coming from the source and diffusing toward the interface, whereas defender walkers will tend to diffuse from the interface toward the sink. Alternatively, we can envision the relaxation process in the defender as being one in which "holes" diffuse from the sink toward the interface. If the holes are considered to be walkers, then we have a process that begins to have some of the features of diffusion-limited aggregation (DLA),[17,18] where the growth of the interface depends on both the arrival of the hole at the interface and on the sticking probability of the hole once it reaches the interface.

The challenge is to define the rules which apply to the walkers as they interact at the invader/defender boundary; this is similar to the sticking probability of DLA—the interaction of walkers with the interface when they reach the surface of the aggregate.[19] The availability of two types of walkers, one for the invader and one for the defender, provides a fundamental and elegant basis for defining a dynamic "surface evolution probability." Consider two neighboring sites spanning the interface. The evolution of the surface is clearly a two-site interaction: the states of

the sites on both sides of the interface are crucial to the propagation of the front. Hence, we obtain for the interface growth I_G the form $I_G = \alpha D_i H_d P_i + \beta D_d H_i P_d$ where H is the hole density. It is this equation which provides us with the necessary connection between the pressure fields P_d and P_i at the interface.[3] Then, depending on the model desired, α and β can be given appropriate values. For example, if $\beta = 0$, the invasion process can only move forward, even at the microscopic level. With the flexibility of the coefficients α and β, one can invoke a variety of microscopic models which go beyond those suggested by the hydrodynamic view of interfacial growth.[4]

The foregoing arguments provide a conceptual relationship between the DLA process and the treatment of fluid flow invasion via two armies of random walkers. It may be worthwhile pointing out that our treatment of the fluid displacement process is formally analogous to a diffusion-limited chemical reaction process[25,26] occurring along an interface where the reaction rate is simply the product of the concentrations multiplied by the "reaction coefficient" D_i. The statement in the usual DLA process is that the diffusion rate of the invader species is large with respect to the diffusion rate of the defender. It is clear that our expression reduces to the usual DLA boundary condition when the limit of high invader diffusivity is taken.

[3] It is interesting to replace each hole density in I_G by the equivalent population density expression, $H = 1 - P$, to obtain $I_G = \alpha D_i P_i + \beta D_d P_d - (\alpha D_i + \beta D_d) P_i P_d$. With an appropriate choice of the coefficients, $\alpha = \beta$ (the negative sign denotes the direction of interface motion), and setting $D_i = D_d = D$, one obtains the expression $I_G = D(P_i - P_d)$, so that evolution of the front would be in terms of the population difference to first order in pressures. This is consistent with the form one might expect from hydrodynamics and is a common choice for such simulations,[20,21] although generalizations to higher powers have been considered.[22,23] However, if $D_i \neq D_d$, then one should expect the evolution of the front to be governed by $I_G = \alpha[(D_i P_i - D_d P_d) + (D_i - D_d) P_i P_d]$, where the nonlinear term explicitly couples defender and invader populations.[24]

[4] It has been observed that growth is also proportional to the "average" interface curvature. This feature is inherent within the discrete entity simulation. Once the system has evolved for some time, the defender density of walkers approaches unity (the bulk relaxation time is long compared to interfacial growth times, and unity is the greatest achievable density). It is well known that the random walk solves Laplace's equation. Thus, consider a fixed interface with a radius of curvature R (fingering into the defender phase) held at a fixed defender pressure P_d along the interface. Ignoring contributions to the pressure field from distant surface locations (these are temporally retarded anyway), the solution to Laplace's equation of a site near the interface in the defender phase could be represented as an expansion in the curvature parameter $\kappa = 1/R$. Namely, $P_d(r) \approx P_0(r)[1 - \alpha(r)\kappa + O(\kappa^2)]$, where $P_0(r)$ is the solution to Laplace's equation for $\kappa \to 0$, and $\alpha(r)$ is an r-dependent function. By virtue of the random walk process, this solution (to all orders in κ) is obtained by our simulation. The hole density in the defender phase a unit distance away from the interface is then $H_d \approx \nabla P_0 + \kappa \nabla \alpha(r)$, where the gradients are evaluated at the interface. Thus, the interfacial growth has contributions from both the pressure gradient and surface curvature.

We can now see how the simulation recognizes the two different time scales of the physical problem. One time scale is associated with the surface, i.e., the development of the invaded network, which occurs over periods of one simulation step, and the other time scale is associated with the relaxation of the pressures at the nodes of this invaded network. This relaxation occurs over periods of order L^2 simulation steps, where L is the system size and is just the time for a random walker to span a distance L. The simulation we present here explicitly separates the two time scales. The evolution of the surface is controlled by the pressures of the two phases at the interface, whereas the relaxation of the bulk pressures is controlled by the diffusivity of the walkers. Several limiting cases exist. If the diffusivities of the defender and invader walkers are large, such that the bulk pressures have time to relax between each pore/throat invasion, the process becomes one dominated by percolationlike behavior. In this case, as long as both diffusivities are large, the transients within the bulk regions of defender and invader are unimportant. On the other hand, in the event that the invasion time scales and relaxation time scales are equivalent, the dynamics within the bulk regions of defender and invader dominate due to the invasion occurring at a surface, and the bulk relaxation occurring within a volume. In this event, the viscosity ratio of the two fluids is important as well, controlling the invasion pattern: stable displacements (where only the defender phase relaxes quickly) to viscous fingering displacements (where only the invader phase relaxes quickly).

3. METHODOLOGY

We carry out a simultaneous walk of a collection of identical random walkers, which closely approximates the process of moving each walker one at a time. Some care must be exercised in this connection, since walkers walking simultaneously must interact in some manner (we drop terms of third order and higher in the walker density). The approximation made has been observed to have no effect on test problems,[27] and the reduction in computational effort relative to the sequential movement of many walkers is certainly advantageous. Further, in order to mimic a defender phase, we introduce a second type of walker to represent the defender phase.

At any time during the displacement all sites are considered occupied by either invader fluid or defender fluid. Some of the sites are occupied by walkers as well as fluid. Initially, all of the lattice sites are occupied by the defender phase. Some of these sites are also occupied by defender walkers; this occupancy generates an initial average defender density for the lattice; in the cases reported below, of 0.5 walker per lattice site. The invader phase

is then introduced at the source. Each site on the source line belongs to the invader phase, and has an invader walker occupancy probability of 0.5. As the displacement progresses, the defender phase is displaced from interior sites, which become occupied by the invader phase. The sink line is kept at an invader walker density of zero and a defender walker density of 0.5.

Walkers within the bulk medium are conserved. This condition was introduced to reduce complexity in the initial study, but it could be modified to explicitly incorporate the "work" done as invader walkers perform displacements as new sites are invaded. In the present study the rules imposed on the walkers are as follows:

(a) Walkers are allowed to migrate to nearest-neighbor sites in the lattice not presently occupied by another walker. This "single-walker-occupancy" rule holds for both the invader walker and for the defender walkers, together and separately.

(b) Walkers that step onto the sink or source line are removed, and these lines are then randomly repopulated at the desired density each time step.

(c) Defender walkers may only step onto those sites that have *never* been visited by invader walkers. This asymmetry in the behavior of the defender and invader walkers means that once a site has been visited by an invader walker, it cannot be reclaimed by the defender species. It should also be emphasized that the diffusivities of the two walkers need not be the same.

In addition to the walker rules, there is a single "rule" involving the fluid phases within the network, which is an accounting process to keep track of the invaded network. This rule for fluid displacement is that when an invader walker steps onto a defender phase site presently unoccupied by a defender walker [as allowed by rule (a)], the defender fluid is assumed to be displaced and the site is then considered to be an invader phase site.

The asymmetry of rule (c) is manifested by the observed fingering patterns and in the trapping of defender walkers. Trapping results when invader walkers have visited all sites surrounding a group of defender walkers: since the defender walkers are forbidden to walk across the path of invader walkers, they are forever isolated. The result inherent within this trapping mechanism is that the trapped defender region is compressed until the region has a 100% defender walker occupancy per trapped site. For example, if the lattice was initialized with a defender walker occupancy of 50%, a region of trapped defender sites might only have one-half of these sites occupied by defender walkers. In the cases we have examined the compression is rarely this severe, since the density of defender walkers at the

invader fluid front is usually quite high, near 100%, even for an initial defender density of 50%.

It should be emphasized that these trapping rules are entirely local, removing the primary inefficiency of many previous approaches. Further, such simple rules also can be efficiently "bit coded." All that is needed is to associate with each site three bits. One of the bits is initially set to zero throughout the lattice (denoting defender phase sites) and is then set to one if an invader walker walks on the sites (denoting invader phase sites). Sites with this bit set to one are then inaccessible to the defender species. The other two bits for each site represent the presence of a defender walker or an invader walker. If either of these is set to unity, the presence of a random walker is known. These set bits are what randomly walk around on the network according to the rules discussed above.

4. RESULTS

(i) *Evolution of a Front:* Figure 1 displays a time series of the resulting structures from the simulation. The initial defender ant density is 0.5 defender walker per lattice site, and an invader ant density difference of 0.5 walker per site is imposed across the network. The underlying network is a 128×128 square lattice, with a source edge and a sink edge with

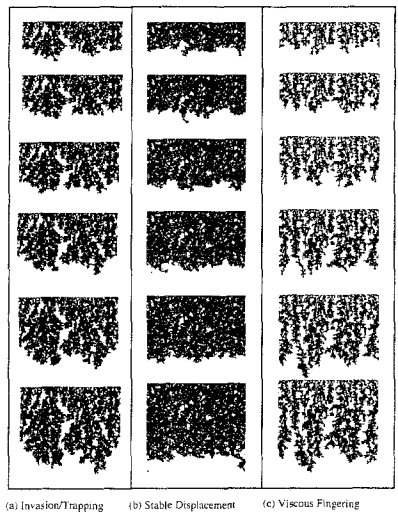

Fig. 1. A series of snapshots showing the invader structure at times from 2000 to 20,000 simulation steps for different viscosity ratios: (a) equal viscosity, (b) viscosity ratio of 0.1, (c) viscosity ratio of 10. The invasion is from the top down and invaded sites are indicated in black.

periodic boundary conditions applied on the two edges perpendicular to the invader walker source-to-sink gradient. Structures separated temporally by about 5000 simulation steps illustrate the evolution of the front. Figure 1a results from a case where the viscosity ratio of the fluids is equal. It is observed to be relatively uniform, although large-scale instabilities occur. Some fingers of these instabilities eventually touch, leaving behind clusters of trapped defender walkers spanning a large range of sizes. Trapped regions are found to be effectively incompressible, even though the initial defender density is only 0.5.

(ii) *Stability of the Front:* An additional generalization that can be added to the technique is the ability to choose, with some degree of arbitrariness, the defender-to-invader viscosity ratio. This allows for the examination of phenomena ranging from stable displacements, with little trapped defender fluid, to viscous fingering, where much of the defender fluid is trapped. In the case of viscous fingering, the defender fluid is given a very low diffusivity (high viscosity), whereas the invader fluid is given a high diffusivity (low viscosity). For stable displacements, the situation is reversed. A time series for viscous fingering (with a defender-to-invader viscosity ratio of 10) is shown in Fig. 1c and that for a stable displacement (with a defender-to-invader viscosity ratio of 0.1) is seen in Fig. 1b. The stable displacement exhibits a broad, uniform front, with only small regions of trapped defender clusters left behind as the front passes. On the other hand, with viscous fingering, the front is very dendritic, leaving great regions of defender fluid behind.

5. ANALYSIS

Our method of performing an invasion process provides information regarding not only the final, steady-state structures, with their invaded and trapped regions, but also such transient information as the lead position of the invading fluid versus time and the invader and defender walker currents (which can provide the macroscopic conductivity of the invaded network[10]). We are, however, primarily interested in the resulting structures, and for further analysis we shall restrict ourselves to a viscosity ratio of one. For this purpose, we have terminated the invasion process when all lattice sites (up to an arbitrary distance from the sink) have either been invaded by invader or are occupied by trapped defender.

(i) *Trapped Clusters:* We have analyzed the trapped defender cluster distribution. If this were a percolation problem performed at the percolation threshold, this information would give results for two exponents, the size distribution exponent τ and the fractal dimension D_d as

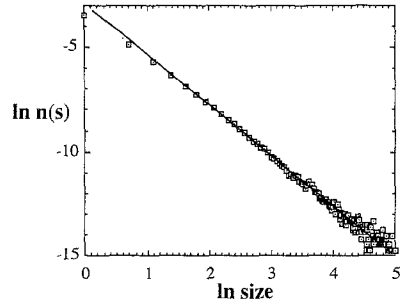

Fig. 2. Frequency distribution of trapped defender cluster sizes plotted against cluster size on a log-log scale. A power-law behavior is observed over several orders of magnitude.

defined by Stauffer.[2] Although this clearly is not a percolation problem in the usual sense of the term, we find, using the above analysis, some quite interesting similarities. The runs to be discussed below have been obtained on three different lattice widths, $L=128$, $L=192$, and $L=256$ lattice spacings. The lengths used for these simulations were, respectively, 300, 375, and 500 lattice spacings in an attempt to minimize the end effects. Once the simulations were completed, a uniformly invaded section of length L was taken to perform measurements.

In Fig. 2 we present the trapped defender cluster size distribution plotted on a log-log scale for the largest lattice. This curve is the result of analyzing structures from 118 simulation runs. Although the lattice is quite small, it appears that the trapped cluster distribution obeys a power law, $n(s) \sim s^{-\tau}$. In order to make a more accurate estimate for the exponent, the results of Fig. 2 are plotted as in Fig. 3 for the quantity $M(s)=$

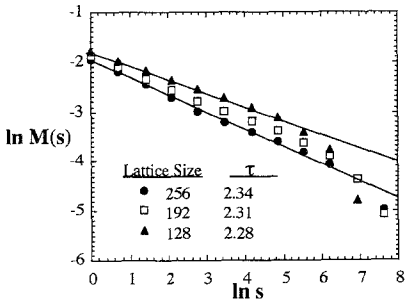

Fig. 3. $M(s)$ as defined in the text plotted against the cluster size on a log-log scale. The power-law exponents are tabulated for three different lattice sizes.

$\sum_{s'=s}^{2s-1} s'n(s')$, which scales as $M(s) \sim s^{-(\tau-2)}$, giving a more accurate determination of the exponent τ. Results for the exponents are determined by a simple fit of the linear regions, and for three lattice sizes are $\tau = 2.28$, 2.31, and 2.34, for the smallest to largest lattices, respectively. The results indicate that over the range of cluster sizes shown for a given lattice, a power-law scaling is quite accurate. However, there is no apparent scaling of the exponent τ with the lattice size to indicate the exponent for an infinite lattice. These values are in strong disagreement with the value $\tau = 2.05$ at the two-dimensional percolation threshold. Continuing with the analogy to percolation, we recall that both above and below the percolation threshold there is an additional exponential decay factor multiplying the power law cluster distribution.[2] If our cluster distribution has this factor as well, the constant in that exponent must be quite small, since no effect is observed in the data up to cluster size $s = 128$. An additional complication in the percolation analogy is that the exponent τ should decrease on either side of the percolation threshold[3]: we find a larger value of τ, which is, in fact, increasing with lattice size! If this problem were in the class of percolation problems, it would only be with increasing dimensionality that the exponent should increase, for example, to a value of 2.5 for dimensions $d \geqslant 6$.[2]

One other quantity that is easily examined is the radius of gyration for the trapped defender clusters. According to Stauffer,[2] the radius of gyration for finite percolation clusters should scale as $r \sim s^{\rho}$, where ρ is an exponent having the value $48/91 = 0.527$ at the percolation threshold, 1/2 above the threshold, and roughly 2/3 below the threshold in two dimensions. The distribution we have measured is shown in Fig. 4 for the largest lattice size. Within the linear region, the exponent is roughly $\rho \sim 0.599$. The smaller lattices, $L = 128$ and $L = 192$, give exponents of 0.58 and 0.592, respectively.

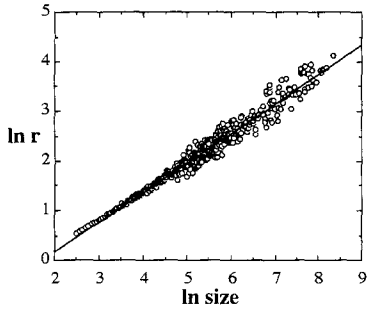

Fig. 4. Average radius of gyration for clusters of a given size are plotted on a log-log scale. This also follows a power-law with an exponent $\rho = 0.599$ for an $L = 256$ lattice.

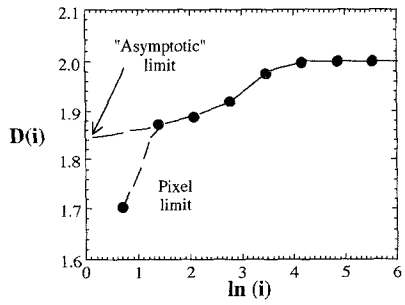

Fig. 5. Fractal dimension $D(i)$ of the invader network vs. window size i.

These values seem to show a weak tendency toward the value of 2/3; however, the accuracy is much too low to make any strong conclusions.

(ii) *Fractal Dimension of the Invaded Structure:* Finally, we can make a direct measurement of the fractal dimension of the network swept by the invading fluid. The problem presented here can be placed on a continuum of viscosity ratios, with one end representing viscous fingering invasions, and the other end representing stable displacements. The invaded network of a stable displacement clearly has a dimensionality of 2, whereas the network of a viscous fingering invasion has a fractal dimension of 1.4–1.7.[28] How does the fractal dimension change with the viscosity ratio? This simulation checks the equal-viscosity limit. We have applied a covering method of analyzing fractal dimensions D using local slopes,[29] and the results are shown in Fig. 5. There is considerable structure to this curve; for large covering squares the trend of $D(i)$ toward two simply reflects the boundary effect and as the window size approaches the pixel limit,[30] the dimensionality drops sharply. Between these two extremes the covering squares tend to suggest a fractal dimensionality $D(i)$ approaching a limit D of about 1.84.

6. CONCLUDING REMARKS

We have presented a generalization of discrete entity simulation methods based on a microscopic, physical behavior which qualitatively agrees with the experimentally observed complex macroscopic behavior. Phenomena such as defender fluid trapping and arbitrary viscosity ratios have been incorporated. We have analyzed these trapped defender clusters in analogy to percolation concepts. The cluster size distribution demonstrates good agreement with a simple power law. In the case of equal

viscosities on a two-dimensional network, we present several predictions for trapped cluster distribution exponents, including the exponent for the radius of gyration, and fractal dimensions.

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