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**Modification of Chemical and Physical Factors in
Steamflood to Increase Heavy Oil Recovery**

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By
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ABSTRACT

Thermal methods and particularly steam injection, are recognized as the most promising for the efficient recovery of heavy oil. Despite significant progress, however, important technical issues remain open. Specifically, still inadequate, is our knowledge of the complex interaction between porous media and the various fluids of thermal recovery (steam, water, heavy oil, gases and chemicals), while the interplay of heat transfer and fluid flow with pore- and macro-scale heterogeneity is largely unexplored.

The objectives of this contract is to carry our fundamental research in heavy oil recovery in the following areas: displacement and flow properties of fluids involving phase change (condensation-evaporation) in porous media; flow properties of mobility control fluids (such as foam); and the effect of reservoir heterogeneity on oil recovery. The specific projects are motivated by and address the need to improve heavy oil recovery from typical reservoirs as well as less conventional fractured reservoirs.

This report covers the work performed in these three areas in the past year. In the area of vapor-liquid flow we present a theoretical and numerical study of steam injection in a pore network. We characterize the displacement in terms of an effective mobility ratio and heat transfer parameters. Displacement patterns are identified in the parameter space. In another study we discuss the problem of steam injection in fractured systems using visualization with micromodels. The interplay of drainage, imbibition and bubble growth is visualized. Conclusions are reached regarding the potential for steamflooding fractured systems. A third study focuses on the development of a pore-network model for foam formation and propagation in porous media. This model, for the first time, accounts for the fundamental mechanisms of foam propagation at the microscale and leads to the determination of various parameters that are currently treated empirically. The effect of viscous forces in displacements in heterogeneous media is described in two separate studies, one involving an extension of percolation theory to account for viscous effects, and another discussing the effect of geometry in general displacement processes. The latter identifies two different regimes, based on the magnitude of the aspect ratio. Effects of correlated heterogeneity are discussed in a study where the characteristics of Invasion and Gradient Percolation in a correlated pore network are explored. Finally, we conclude with a study on the identification of the pore-size distribution from mercury porosimetry using percolation theory.

1 Pore Network Studies of Steam Injection in Porous Media

C. Satik and Y. C. Yortsos

1.1 Introduction

Flows in porous media that involve liquid-to-gas phase change occur in many problems of interest. The phase change can be brought about by one of two mechanisms: 1. Mass Transfer – as in cases where phase change occurs by solute diffusion, and the supersaturation is supplied by pressure reduction (see Li and Yortsos^[3, 4, 5]). 2. Heat Transfer – as in cases where the gas phase growth is externally controlled by the rate of heat supply (see Satik and Yortsos^[6]). The latter include steam injection for oil recovery (Prats^[7]), flows in geothermal systems (Schubert and Straus^[8], Straus and Schubert^[9]), and heat pipes (Ogniewicz and Tien^[10], Udell^[11, 12]). In this chapter we consider the second problem with emphasis on steam injection in porous media.

As with other porous media processes, this problem can be studied at three different levels: 1. The single-pore level, where the emphasis is on condensation and displacement, film and corner flows, wetting phenomena and the distribution of phases within single pores. 2. The pore-network level, where the emphasis is on the integration of events in an ensemble of pores, where pore network topology is predominant. 3. The continuum level, where the emphasis is on the average behavior of the system in terms of variables such as heat fluxes, temperature and saturation levels.

Past efforts have addressed the continuum level, where pore-space events are lumped into relative permeability and capillary pressure functions imported from the isothermal, immiscible displacement literature (e.g. Udell^[12], Sanchez and Schechter^[13], Parlar et al.^[14], Stubos et al.^[15]). These functions are independent of the rates of heat transfer. In contradiction with the assumed analogy with isothermal displacements, however, residual saturations are assumed negligible. This is also the typical approach in the large-scale simulation of steam injection. Experimental investigations have mostly focused on macroscale quantities. Thus, although fundamental to a variety of applications, the underlying mechanisms at the pore- and pore-network levels are still poorly understood. The latter include the configuration of vapor and liquid phases within networks of pores, and the role of heat transfer and phase change.

In isothermal drainage displacements, the displacement patterns depend on the viscosity ratio, M , and the capillary number, $Ca = q\mu/\gamma$, where q is injection velocity, μ is viscosity and γ is the interfacial tension. Lenormand^[16] has identified three distinct regimes: A capillary-control regime, described by Invasion Percolation, where the interface advances by

occupying the perimeter pore throat with the smallest capillary barrier, and two viscous-control regimes, one of Viscous Fingering (large M), that can be described by *DLA*, and another of a Compact (Piston-Like) pattern (small M), described by *anti-DLA*. If steam injection were amenable to the same description, as conventionally assumed, the residual saturations would be relatively large, due to the unfavorable mobility ratio. This is in contrast to experimental observations in steam displacements, where residual saturations are found to be very small. The main reasons for this inconsistency must be sought in the heat transfer and phase change that accompany steam injection processes.

To understand the effect of heat transfer on the steam injection invasion patterns requires an analysis at the pore-network scale. This can be accomplished by a pore-network simulator. To interpret the numerical results to be obtained, however, a theory must be also developed. For this purpose, it is useful to analyze, first, the predictions of macroscopic analyses of steam front stability. Even though at a macroscopic level, these contain important information, which cannot be simply obtained from the available 1-D steam propagation models (e.g. Marx and Langenheim^[17], Mandl and Volek^[18], Yortsos and Gavalas^[19, 20]). For example, in the standard problem of immiscible displacement in porous media, an analysis of the macroscopic stability condition at long waves identifies the condition $M = 1$ as the one that separates viscous fingering and compact regimes, while it also shows the increasing dominance of capillarity at smaller scales (wavelengths) (e.g. Peters and Flock^[21], Yortsos and Hickernell^[22]). These are qualitatively consistent with the pore-scale predictions, for example as described in Lenormand's phase diagram^[16].

Early attempts to model steam injection at the porescale were made by Parlar and Yortsos^[23] who applied percolation theory in a Bethe tree lattice, and by Satik and Yortsos^[24], who modeled slow (quasi-static) growth using percolation concepts and also included nucleation. However, both these studies were limited to very low superheats, where heat transfer is negligible and capillarity predominates. This assumption is likely to fail in many applications. For further progress, a detailed simulator that accounts for capillarity, viscous forces in both phases and heat transfer by conduction and convection is needed. Pore-network simulation has been very useful for the understanding of displacements in porous media^[25]. In the context of phase change, however, it was only recently used (by Li and Yortsos^[4, 5] and Satik et al.^[26], in a study of bubble growth in porous media, and by Satik^[27] and, Satik and Yortsos^[6], in boiling in porous media). The heat transfer-driven process of interest to this chapter shares common mechanisms with the latter process. These will be extensively explored below.

The chapter is organized as follows: First, we present a theoretical analysis using predictions from studies of the macroscopic steam front stability. This theory identifies the effective mobility value as well as the effect of heat transfer on the long-wave stability of the steam front. Then, a pore-network analysis is presented, where the displacement patterns expected to dominate at various conditions are identified. Effects of condensation and heat transfer are particularly emphasized. Subsequently, we present a pore-network simulator that describes steam injection in porous media. The simulator is used to test the basic aspects of the theory. Preliminary experiments of steam injection in glass micromodels are also

reported. Experiments and simulations support qualitatively the theory derived. Finally, implications to relative permeabilities and macroscopic modeling are discussed.

1.2 Theory

1.2.1 Macroscopic Scale

The problem considered is displacement of liquid water by steam in a horizontal geometry. Gravity effects are neglected, our main objective being the investigation of heat transfer and condensation effects. The steam front stability was first analyzed by Miller^[28], and was later extended by Yortsos^[29] to account for lateral heat losses. Miller's^[28] stability condition at long waves can be rearranged to read as follows

$$M_c = \frac{q_s}{q_w} \left[1 + \frac{(1 + M^*)St}{(1 + St)Pe} \alpha_D \right] + O(\alpha_D^2) \quad (1)$$

where, $M = \mu_w/\mu_s$ is the ratio of viscosities, subscript c indicates stability, q_i is the volumetric velocity per unit area of phase i , $M^* = M\rho_s/\rho_w$ is the ratio of the kinematic viscosities, $St = C_{pw}\Delta T/L_v$ is the Stefan number, the wavenumber α_D was made dimensionless with $k^{1/2}$, and we defined the effective Peclet number

$$Pe = \frac{k^{1/2}\rho_s C_{pw} q_s}{\lambda} \quad (2)$$

based on the pore scale $k^{1/2}$. The latter expresses the relative importance of convection over conduction at the pore scale. For the particular application of Miller's^[28], the ratio of velocities reads

$$\frac{q_s}{q_w} = \frac{1 + A}{1 + \frac{\rho_s}{\rho_w} A} \quad (3)$$

where

$$A = \frac{(1 - \phi)\rho_r C_{pr} St}{\phi\rho_s C_{pw}(1 + St)} \quad (4)$$

The displacement is stable or unstable, depending on whether M is smaller or larger than M_c , respectively. Equation (1) reveals the following:

1. Condensation stabilizes the front and reduces the effective mobility ratio by the factor q_s/q_w . From (3)-(4), the latter increases with an increase in A , namely with an increase in St and the ratio of solid-to-fluid heat capacities, and with a decrease in the density ratio, ρ_s/ρ_w . Inversely, evaporation increases the effective mobility ratio by the same factor. These conclusions were also reached by Zazovskii^[30].

2. Heat conduction exerts a stabilizing influence, which increases as the front curvature increases (larger α_D). This heat transfer effect is shown to be proportional to $StPe^{-1}$. The

effect is somewhat similar to capillarity, which, however, was not considered in Miller's^[28] analysis (see also below). In isothermal displacements, capillary effects enter at the same order as heat transfer, and they are also stabilizing (e.g. Peters and Flock^[21], Yortsos and Hickernell^[22]).

By drawing an analogy with isothermal, immiscible displacements, we may postulate from the above that the parameters controlling the displacement patterns in steam injection, and more generally in external displacements involving phase change, would be an effective viscosity ratio,

$$M_{eff} = \frac{M(1 + \frac{\rho_s}{\rho_w} A)}{1 + A} \quad (5)$$

the heat transfer-condensation group, $StPe^{-1}$, and the capillary number, $Ca = \frac{q_s \mu_w}{\gamma}$. Further understanding of the displacement patterns, however, requires consideration of a pore-network scale analysis.

1.2.2 Pore-Network Scale

As previously noted, isothermal drainage displacements are described by three limiting regimes, a capillary-control and two viscous-control regimes, depending on the values of Ca and M (Figure 1). In steam injection, which is a non-isothermal drainage involving phase change, we expect an additional regime to develop when heat transfer dominates over capillary or viscous forces. The presence of the additional heat transfer parameter, $StPe^{-1}$, leads to an extension of Lenormand's^[16] phase diagram to a three-dimensional space. Furthermore, heat transfer and phase change will modify the boundaries of the displacement regimes. A detailed theory of these effects will be presented elsewhere. Here, we describe the qualitative effects and use the pore-network simulation for quantitative results.

a. Heat-transfer Control ($StPe^{-1} \gg 1$) Consider the case when heat transfer dominates. To characterize the displacement pattern at these conditions, we consider material and energy balances across any meniscus I at the front (Figure 2)

$$\rho_s(u_{sI} - v_I) = \rho_w(u_{wI} - v_I) \quad (6)$$

and

$$\rho_s L_v(u_{sI} - v_I) = -\lambda \frac{\partial T}{\partial n} \parallel_I \quad (7)$$

where all velocities are components in the normal direction n . Solving for v_I , we find

$$v_I = u_{sI} + \frac{\lambda}{\rho_s L_v} \frac{\partial T}{\partial n} \parallel_I \quad (8)$$

Figure 1: Schematic of phase diagram of drainage.

In the absence of viscous or capillary effects, the steam velocity u_{sI} is uniformly distributed at the perimeter sites, hence the front velocity would be controlled by the net heat transfer from the steam to the liquid region (second term on the *RHS* of (8)). Under these conditions, and when conduction dominates, we expect the corresponding displacement pattern to be compact (e.g. similar to a melting pattern), as conduction would stabilize any protruding front movement. This problem is similar to the piston-like displacement obtained at favorable mobility ($M \ll 1$) in isothermal drainage and can be described by the *anti-DLA* algorithm. From a dimensional analysis of (8), the conditions for this pattern read $StPe^{-1} \gg 1$. It should be added that convection may also affect this pattern, but in a way that is presently unclear and which needs to be studied further.

We conclude that at conditions of heat transfer control, a compact pattern is possible, despite the large value of M in steam injection, which in the absence of capillarity would indicate a viscous fingering pattern. The compact pattern is largely responsible for the low residual saturations associated with steam displacements. This limiting pattern complements the other two limiting patterns for this case of large M , namely Invasion Percolation at capillary control, and Viscous Fingering at viscous control (Figure 3). Heat transfer and phase change would also affect the boundaries of the latter two patterns as qualitatively described below. A more quantitative analysis will be presented elsewhere. We recall that the various transitions from the capillary to the viscous fingering regimes have been studied by Lenormand^[16].

Figure 2: Schematic vapor-liquid interfaces during steam injection in porous media.

Figure 3: Schematic of phase diagram for steam injection.

b. Effect on the Percolation Regime Consider an Invasion Percolation pattern at conditions of capillary control. In the absence of viscous and inertia effects, the front advances by penetrating the throat at the steam perimeter with the least capillary resistance (e.g. that with the largest radius, denoted by A in Figure 2), following standard Invasion Percolation rules. Menisci in all other throats (such as B in Figure 2) will stay stationary (or oscillate slightly). Thus, during a penetration step, the meniscus velocity v_I is negligible in all pores, except pore A , where growth occurs. From (6)-(7), the liquid velocity adjacent to any pore B is

$$u_{wB} = -\frac{\lambda}{\rho_w L_v} \frac{\partial T}{\partial n} \parallel_B \quad (9)$$

while that adjacent to pore A is

$$u_{wA} \approx u_{sA} + \frac{\lambda}{\rho_s L_v} \frac{\partial T}{\partial n} \parallel_A \quad (10)$$

which can be further rearranged to read

$$u_{wA} \approx \frac{Q_s}{\pi r^2} - \frac{1}{\rho_s L_v} \left(-\sum_I \lambda \frac{\partial T}{\partial n} \parallel_I \right) \quad (11)$$

Here, Q_s denotes the volumetric steam injection rate, the sum over all perimeter menisci represents the net heat transfer from the steam zone to the liquid and solid, and it was

assumed, for simplicity, that heat transfer from the steam to the solid is negligible. Equations (9)-(11) show the following:

1. The liquid velocity in sites B , where menisci are stationary, is not zero, as is the case in isothermal displacements, reflecting the possible steam condensation. It follows that the viscous pressure drop in the liquid between site B and the growth site A would be smaller than in the isothermal case.

2. The liquid velocity at the growth site A is also smaller than in the isothermal case, due to the net heat transfer and the phase change.

Both of these effects would result in a decrease of the viscous pressure drop that develops in the liquid between the growth site A and any other perimeter site B , thus in an increase of the region where capillarity dominates. The net effect is equivalent to a reduction of the effective viscosity ratio, in analogy to the macroscopic expression (5). Quantitative conditions, however, will be derived elsewhere.

c. Effect on the Viscous Fingering Regime Consider, next, the case of viscous control. In the absence of capillary effects, the front advance is controlled by the velocity field in the liquid and by the associated heat transfer

$$v_I = u_{wI} + \frac{\lambda}{\rho_w L_v} \frac{\partial T}{\partial n} \parallel_I \quad (12)$$

where use was made of (6)-(7). Under viscous fingering conditions, the isotherms in the liquid will be quite steep near the finger tip, resulting into large heat transfer rates at sufficiently large $StPe^{-1}$, as can be seen from a dimensional analysis of (12). The front velocity would be accordingly reduced, leading to a departure from the viscous fingering pattern towards a more compact pattern. The overall effect would be to reduce the size of the viscous fingering regime in the associated phase diagram.

Based on the above theoretical considerations, we conclude that heat transfer and phase change at the pore-network scale may significantly influence the displacement patterns, hence the overall flow behavior, in steam injection. In particular, the compact pattern identified at conditions of heat transfer control is consistent with the commonly accepted high displacement efficiency and low residual saturations in steam injection, while the reduction of the effective mobility ratio due to condensation reduces significantly the tendency for viscous fingering associated with the large M of a gas-liquid displacement.

1.3 Pore-Network Simulations

Subsequently, pore-network simulations were conducted to test the above theory. In these models, the porespace is approximated by a network of sites (pores) and bonds (throats) of various sizes randomly distributed. For the problem of heat transfer in porous media one additionally needs to discretize the solid. For this purpose, a square network of solid

Figure 4: Pore space and solid space lattice representation in the numerical simulation.

sites and bonds, complementary to that of the porespace, was constructed to account for heat capacity and heat conduction in the solid matrix, respectively. A schematic of the two lattices is shown in Figure 4. The key elements of the algorithm used are as follows:

1. Variables, such as pressure and temperature, are assigned to sites (pores or solid sites) only. They represent lumped variables, volume-averaged over the respective site volumes (much like a finite-differencing scheme). Vapor-liquid menisci reside in sites at the cluster perimeter, whose occupancy by vapor may be partial or complete, as determined from fluid flow and heat transfer.

2. Pore throats provide the capillary pressure barrier to the motion of the menisci and also control transport. A pore throat is invaded when the capillary pressure across the meniscus in that throat exceeds for the first time the capillary barrier

$$P_{si} - P_{wj} = 2\gamma\mathcal{H}_{ij} \quad (13)$$

where i and j denote adjacent sites at the cluster perimeter and $\mathcal{H}$ is the throat mean curvature (equal to $1/2r_{ij}$ for a cylindrical throat).

3. The pressure field is solved from mass and momentum balances. For a site not in the steam front, the continuity equation was discretized as follows

$$\sum_j A_{ij} u_{i \rightarrow j} = 0 \quad (14)$$

where A_{ij} is the cross-sectional area connecting adjacent sites i and j and the summation is done over all sites j (4 for square lattices). For liquid-filled or vapor-filled sites in the perimeter, (14) was modified to also account for vaporization or condensation. Assuming creeping flow in the absence of gravity, the equation for the flow velocity from i to j is $u_{i \rightarrow j} = \frac{G_{ij}}{\mu} \left[\frac{P_i - P_j}{l} \right]$, where G_{ij} is the flow conductivity (in general a geometric parameter), l is the bond length, P is pressure, and pressure drops were assumed associated with throats only. For viscous (Poiseuille-type) flow in a capillary, $G_{ij} = \frac{r_{ij}^2}{8}$. These equations apply to both the liquid and the vapor. It must be pointed out that in the steam injection problem it was also necessary to solve for the pressure field in the vapor phase, despite its low viscosity.

4. Heat transfer by conduction and convection in the liquid phase, and by conduction in the solid phase, was simulated. Sufficiently fast heat transfer is assumed for the gas phase, so that its temperature is spatially uniform. In the liquid-occupied lattice, the energy equation

$$\rho_w C_{pw} \left[\frac{\partial T_w}{\partial t} + \mathbf{u}_w \cdot \nabla T_w \right] + \nabla \cdot \mathbf{q}_w = -\alpha_{rw}(T_w - T_r) \quad (15)$$

was discretized by assigning T_w to the sites of the porespace lattice, T_r to the sites of the solid lattice, and expressing the conductive heat flux as $q_{w,i \rightarrow j} = \lambda_w \frac{(T_{w,i} - T_{w,j})}{l}$ for throats joining sites i and j . Solid-liquid heat coupling is expressed through the heat transfer coefficient, α_{rw} , which was taken as *constant*. The coupling is assumed to occur over the four corner pore bodies surrounding a solid lattice site. The energy balance in the solid

$$\rho_r C_{pr} \frac{\partial T_r}{\partial t} + \nabla \cdot \mathbf{q}_r = -\alpha_{rw \text{ or } rs}(T_r - T_{w \text{ or } s}) \quad (16)$$

was discretized in the solid lattice, with conductive heat fluxes approximated by $q_{r,i \rightarrow j} = \lambda_r \frac{(T_{r,i} - T_{r,j})}{l_r}$, where λ_r is solid conductivity and l_r is a length scale of the solid "grain" (also assumed constant). Heat conduction in the solid occurs through the bonds of the solid lattice, which "bridge" adjacent solid grains (sites). Heat transfer at the vapor-solid interface was assumed much weaker than the solid-liquid coupling ($\alpha_{rs} \ll \alpha_{rw}$) and was neglected.

5. Across any meniscus, local phase equilibria are assumed, so that the Clausius-Clapeyron equation $P_{si} = P_{vo}(T_s)$ applies, where P_{vo} is the saturation pressure.

6. The liquid phase may be trapped by the expanding gas cluster. In the numerical algorithm, the volume of the trapped liquid is taken as constant, since the ratio of liquid to vapor densities is large.

The simulator calculates the net molar influx to the vapor phase, $\frac{dn}{dt}$, by accounting for injection as well as possible condensation at the vapor-liquid perimeter sites. This rate determines the changes in the pressure or volume of the steam zone via an equation of state (here taken to be the ideal gas law),

$$\frac{d}{dt} \left(\frac{P_s V}{T_s} \right) = R \frac{dn}{dt} \quad (17)$$

where R is the ideal gas constant and V the steam zone volume. Whether the steam zone grows ($dV > 0$), and at which perimeter site (pore-filling step), or the interface remains fixed while the pressure increases ($dP_s > 0$) (pressurization step), depends on whether or not capillary condition (13) is satisfied at the perimeter. If none of the perimeter capillary barriers is reached, the interface remains stationary and the steam pressure P_s increases at a constant volume. When (13) is satisfied for the first time across a perimeter throat, a rheon event occurs, invasion of the site adjacent to that throat begins and the pore-filling step commences. During this step, we neglect the capillary pressure in the invaded sites. The liquid is then displaced from the invaded site(s), and both vapor volume and pressure (or temperature) can vary as determined from the heat transfer and fluid flow calculations. Under certain conditions, for example when the steam zone is sufficiently large, multiple sites may be invaded (and filled) at the same time, in which case pore-filling in each pore is calculated incrementally in small time steps. The entire pressure and temperature fields are needed to determine pore throat penetration and pore-filling, and although pressure drops are not large, they must be computed to account for convection and viscous forces. A Successive-Over-Relaxation scheme was used for the numerical solution, while iterations on the time increment is necessary for a satisfactory convergence of the algorithm.

The above equations give rise to the previous dimensionless numbers, M , Ca , St , and Pe , to the dimensionless heat transfer coefficients, $d_{rw} = \frac{\alpha_{rw} l}{\pi r^2 \lambda_r}$ and $d_{rs} = \frac{\alpha_{rs} l}{\pi r^2 \lambda_r}$ and the ratio of thermal conductivities $\kappa = \frac{\lambda_r}{\lambda_w}$. In the following, various simulations will be conducted to analyze the sensitivity of the process to some of these parameters.

1.4 Simulation Results

In the simulations presented below, throat sizes were randomly assigned from a uniform distribution, while pore body sizes were kept constant. In the absence of better information, geometric parameters, such as the throat mean curvature and flow conductivity were approximated by their expressions in cylindrical geometries. The porespace is initially filled with a liquid at an initial temperature of 21 °C, and an initial pressure of 14.696 psi. A constant rate superheated steam at 120 °C is injected on the one side of a rectilinear domain, with no-heat flux boundary conditions imposed on all other boundaries. A constant pressure (14.696 psi) condition is applied on the opposite boundary, with no-flow conditions imposed on all other boundaries. Standard conditions correspond to the following values: $\rho_s = 0.5886 \text{ kg/m}^3$, $\rho_w = 960.85 \text{ kg/m}^3$, $\rho_r = 2082.4 \text{ kg/m}^3$, $\lambda_s = 0.0245 \text{ W/m-K}$, $\lambda_w = 0.6808 \text{ W/m-K}$, $\lambda_r = 6.808 \text{ W/m-K}$, $\mu_s = 1.202 * 10^{-5} \text{ N-s/m}^2$, $\mu_w = 2.4799 * 10^{-4} \text{ N-s/m}^2$, $L_v = 2.2568 * 10^6 \text{ J/kg}$, $\gamma = 0.0584 \text{ N/m}$, $C_{ps} = 2.0289 * 10^3 \text{ J/kg-K}$, $C_{pw} = 4.2092 * 10^3 \text{ J/kg-K}$, $C_{pr} = 8.3732 * 10^2 \text{ J/kg-K}$, $d_{rw} = 0.1$, $d_{rs} = 0.001$, $l = 2500 \text{ }\mu\text{m}$, $R_t^* = 300 \text{ }\mu\text{m}$ and $R_s^* = 750 \text{ }\mu\text{m}$, $\phi = 0.25$. The steam mass injection rate for the base case was taken as

Figure 5: Invasion percolation patterns at two different stages.

$$\dot{m} = 1.2599 * 10^{-6} \text{ kg/s.}$$

For comparison purposes, the Invasion Percolation patterns at two stages of growth are shown in Figure 5. These patterns are obtained directly from an Invasion Percolation algorithm that also includes trapping (Feder^[31]). Here, and in the figures to follow, sites colored with white or black represent liquid-only or vapor-only occupancy, respectively, while gray denotes partial liquid occupancy. The solid lattice is also indicated in white. To be noted also that all throats are shown in black, regardless of their occupancy. We would expect such a pattern to emerge at the limit of capillary control (Figure 3). Figure 6 shows two consecutive snapshots of steam injection for the base case ($Ca = 0.994$, $M_{eff} = 0.1189$, $StPe^{-1} = 0.01241$). The pattern is clearly of the Viscous Fingering type. Contrary to the percolation pattern, here many sites at the front are simultaneously invaded. Figure 7 shows liquid and solid temperatures and the liquid pressure corresponding to the pattern of Figure 6b (at conditions of breakthrough), where black or white denotes maximum or minimum values, respectively. The steam temperature is spatially constant, almost equal in value to the injected, while the steam pressure is the equilibrium vapor pressure corresponding to the injection temperature. The temperature distribution is rather steep and roughly

Figure 6: Fluid occupancy patterns at two different stages of steam injection ($Ca = 0.994$, $M_{eff} = 0.1189$, $StPe^{-1} = 0.01241$).

contours the steam zone as a boundary layer. In contrast, the pressure field is smoother. Clearly, because of the relatively large value of the injection rate used here, heat transfer is limited, and the controlling factor is the viscosity contrast. The solid temperature is shown to be away from equilibrium. This reflects the negligible heat transfer between vapor and solid, assumed in the model. Because of this lack of thermal equilibrium between solid and vapor, the effective viscosity ratio is not reduced to its M_{eff} value, but remains close to M . This is the main factor contributing to the viscous fingering pattern. Figures 8 and 9 show corresponding results as the injection rate is varied. As indicated in the theory, rate affects both Ca and $StPe^{-1}$, hence the pattern is expected to deviate towards a compact or a percolation pattern, depending on the particular values. Figure 8 shows occupancy and temperature profiles at breakthrough for $\dot{m} = 1.2599 \times 10^{-8}$ kg/s, where $Ca = 0.00994$ and $StPe^{-1} = 1.241$. The occupancy pattern is clearly more compact, compared to Figure 6, and although there exists some amount of trapping, the pattern is different than the Invasion Percolation of Figure 5. The corresponding liquid temperature profiles indicate that heat transfer is a strong factor in this displacement. It is interesting to note that the steam

Figure 7: Temperature and pressure patterns corresponding to Figure 6b ($Ca = 0.994$, $M_{eff} = 0.1189$, $StPe^{-1} = 0.01241$): (a) Liquid temperature, (b) Solid temperature, (c) Liquid pressure.

Figure 8: Effect of injection rate on steam injection pattern ($Ca = 0.00994$, $M_{eff} = 0.1189$, $StPe^{-1} = 1.241$): (a) Fluid occupancy, (b) Liquid temperature, (c) Solid temperature.

temperature rapidly decreases inside a thin boundary layer near the inlet to the equilibrium temperature corresponding to the applied outlet (atmospheric) pressure. This was also observed in other simulations, and it is certainly influenced by the constant pressure boundary condition used at the outlet. Solid temperature profiles are smooth and in equilibrium with the liquid (Figure 8c), indicating efficient heat transfer. As a result, the effective mobility ratio is likely to be close to the theoretical expression (5) for this problem. Figure 9 shows results for the case $\dot{m} = 1.2599 \times 10^{-9}$ kg/s, with corresponding values $Ca = 0.000994$ and $StPe^{-1} = 12.41$. This pattern is similar, but not identical to percolation (compare with Figure 5), with substantial trapping and a ramified growth. Liquid and solid temperatures have many of the previous features. The transition towards a pattern with percolation and/or compact displacement features as the injection rate decreases, is consistent with the previous theory and the phase diagram of Figure 3. For more quantitative results, the boundaries of the various patterns need to be quantitatively evaluated. This will be reported elsewhere.

The effect of L_v is shown in Figure 10, where the latent heat was reduced by a factor of 100 compared to the base case (here $Ca = 0.994$, $M_{eff} = 0.0237$, $StPe^{-1} = 1.241$). Comparison with Figure 6 shows that the degree of fingering is substantially suppressed, the displacement tending towards a more compact pattern, although substantial trapping may also exist. One should keep in mind that trapping is accentuated in 2-D displacements. Liquid and solid temperatures have common features with those of Figures 8 and 9, indicating efficient heat transfer. The results are consistent with the theory that predicts tendency away from the viscous fingering pattern as L_v decreases (note that it affects both M_{eff} and St).

Figure 9: Effect of injection rate on steam injection pattern ($Ca = 0.000994$, $M_{eff} = 0.1189$, $StPe^{-1} = 12.41$): (a) Fluid occupancy, (b) Liquid temperature, (c) Solid temperature.

The sensitivity to the latent heat could be of importance at conditions of phase change near the critical point. The approach towards the compact pattern, when heat transfer is controlling, can be verified by varying the liquid conductivity. Contrary to St , which affects indirectly M_{eff} , the liquid conductivity only affects Pe (although it also indirectly influences the solid temperature). Figure 11 shows occupancy and temperature profiles for the conditions of the base case, but with the liquid conductivity increased by a factor of 100 ($Ca = 0.994$, $M_{eff} = 0.1189$, $StPe^{-1} = 1.241$). We observe that now the displacement is quite compact, with some degree of trapping, which, however, is not due to capillarity. The liquid temperature profiles indicate again a boundary layer near the entrance where the temperature falls near the equilibrium value corresponding to the outlet pressure. Solid temperature profiles are smooth, and parallel the liquid profiles, indicating that thermal equilibrium was practically achieved in this case. As pointed out above, this is also beneficial in reducing the effective mobility to its theoretical value (5).

1.5 Discussion

The pore-network simulations show that the general conclusions of the theory regarding the limiting patterns and their dependence on Ca , M_{eff} and $StPe^{-1}$ are valid. They also indicate, however, the importance of thermal equilibrium between solid and fluids. In the simulations, the vapor-solid heat transfer was taken negligibly small, thus the solid tem-

Figure 10: Effect of latent heat on steam injection pattern ($Ca = 0.994$, $M_{eff} = 0.0237$, $StPe^{-1} = 1.241$): (a) Fluid occupancy, (b) Liquid temperature, (c) Solid temperature.

Figure 11: Effect of liquid thermal conductivity on steam injection pattern ($Ca = 0.994$, $M_{eff} = 0.1189$, $StPe^{-1} = 1.241$): (a) Fluid occupancy, (b) Liquid temperature, (c) Solid temperature.

perature is mostly controlled by heat transfer from the liquid. In the absence of thermal equilibrium, as is the case in Figure 6, where rates are high, the front is not sufficiently slowed down to lead to the reduced effective mobility of (5), hence viscous fingering patterns may emerge, due to the highly unfavorable M value. This effect shows the importance of accurate modeling of the solid-fluid heat transfer. In a realistic situation, however, heat losses to the surroundings will further increase condensation at the front, hence leading to yet lower (more stabilizing) values of M_{eff} (see also Yortsos^[29]).

Theory and simulations show the significance of heat transfer in determining the displacement patterns, which ultimately control residual saturations and relative permeabilities. At conditions of strong heat transfer control, in particular, the residual saturation would be negligible, as dictated by a piston-like type displacement. This is consistent with experimental observations. This also suggests that contrary to the conventional assumption, relative permeabilities should depend on the rates of heat transfer, for example through the parameter $StPe^{-1}$. The precise dependence needs to be further investigated.

The above were based on the assumption of negligible gravity and inertia effects. While the former can be estimated reasonably well from existing theories, the latter may exert novel effects. We should point out that in the simulations the maximum value of the local Reynolds number in the vapor zone often exceeded the creeping flow (Darcy) regime. These are currently under study.

Comparison of the theory and simulations with experiments is difficult, primarily due to the difficulty in the control of the heat losses. Preliminary experiments of steam injection in etched-glass micromodels have been conducted in our laboratory (Yortsos^[32]). Because of the heat losses, the steam front was found to advance in an intermittent fashion and to oscillate (see also Kong et al.^[33]). In addition, because of the rather large rates used, the steam flow is likely to be also controlled by inertia effects. The patterns obtained have the general features of drainage, with well-delineated vapor-liquid menisci advancing through rheon events. In many cases, the menisci are stationary, although condensation continues at the front. However, further quantitative comparison with theory and simulations is needed.

The theory developed could be extended to the more important problem of steam displacement of an oil initially in place. This interesting problem would involve simultaneous drainage and imbibition (due to condensed water) or a double drainage mechanism similar to three-phase oil-water-gas flow. This is currently under consideration.

1.6 Conclusions

In this chapter, we presented both a theoretical and a numerical study to determine the patterns expected to develop during steam displacement of water in porous media. Particular emphasis was placed on the roles of heat transfer and condensation, which differentiate steam injection, or other phase-change process, from simple drainage. The theory predicts a twofold effect: the reduction of the effective mobility ratio to values much smaller than the nominal, and the emergence of a compact pattern at conditions when heat transfer

dominates. A corresponding phase diagram with coordinates M_{eff} , Ca and $StPe^{-1}$, where St is the Stefan number and Pe the Peclet number, can be developed. The reduction of the effective viscosity ratio suppresses the tendency for viscous fingering, typically associated with gas-liquid displacements. The existence of the compact regime at conditions of heat transfer control is also consistent with the very small residual saturations, typically observed in steam displacements.

A pore network simulator was next presented. The simulator accounts for viscous and capillary forces in the vapor and liquid, and for heat conduction and convection in the liquid and heat conduction in the solid. Depending on the location in the parameter space, displacement patterns were shown to lie in the compact, percolation or viscous fingering regimes. The theory was found to be in general agreement with the numerical simulations. Furthermore, heat transfer to the solid (and more generally, heat lost to the surroundings) were found to have a significant effect. Poor heat transfer reduces the beneficial effect of the effective mobility lowering and leads to viscous fingering patterns of the type expected in gas-liquid displacements. On the other hand, a decrease in the latent heat and an increase in the thermal conductivity of the liquid lead towards compact patterns. Observations from experiments in micromodels support the general findings.

The results show that the use of a relative permeability formalism to describe the growth of a vapor phase, using concepts borrowed directly from the isothermal displacement literature, must be re-examined to include heat transfer rates. A similar observation also applies to other phase-change processes, such as a condensing gas-drive. Effects of inertia and gravity, which are important in gas-liquid displacements were not included. These, as well as the extension of the approach to the more interesting problem of steam displacement of oil, are currently under study.

2 Visualization and Simulation of Immiscible Displacements in Fractured Systems using Micromodels: Steam Injection

M. Haghighi and Y. C. Yortsos

2.1 Introduction

Steam injection is a potentially effective method for the recovery of heavy oil from reservoirs. There are large accumulations of heavy crude and tar sands recoverable by steam injection in certain parts of the world, especially in Western Canada, Central Venezuela and in California and Utah in the U.S. [34]. Steam injection can also be used to recover light crude, at least as or even more effectively than waterflooding [34]. Naturally fractured reservoir may contain 25-30% of the world supply of oil [35]. Thus, steam injection in fractured reservoirs has a high potential importance in oil production.

Unfortunately, the understanding of steam injection in fractured systems is currently based mostly on phenomenology and typically consists of applying a double porosity formalism to commercial steam simulators [36], [37], [38]. Most of these use capillary imbibition as the key mechanism for the exchange of fluids between the matrix blocks and the fracture network. Such a purely numerical approach offers little to further our insight in the process. As a reasonable alternative, the study of injection (both experimental and numerical) in model geometries that mimic fractured systems was considered. Good candidates are Hele-Shaw cells and glass micromodels. Such special geometries are considered in this research.

2.1.1 Steamflooding in Fractured Systems

Sahuquet and Ferrier [39] carried out a steam-drive pilot in a fractured, carbonated reservoir. They observed increased oil production without early heat or steam breakthrough. They also reported CO_2 generation, which is the result of dissociation of steam with carbonated rocks, which improved the process efficiency.

Dreher et al. [40] carried out some laboratory experiments and reservoir simulation for hot water and steam-flooding in carbonate, fractured rocks. They observed very high oil recovery from the matrix when either hot water or steam was injected into the fractures. CO_2 generation, oil swelling and viscosity reduction were mentioned as enhanced oil recovery mechanisms.

Jensen [37] performed waterflooding and steam injection on sandstone and carbonate fractured cores. He found imbibition as the most important recovery mechanism in fractured sandstone, while thermal swelling and viscosity reduction were the major recovery mechanisms in fracture carbonate cores. He also found changes in the endpoint saturation in fractured sandstones, which tend to the lower final oil saturation (higher oil recovery) in

solid cores compared to fractured cores and to increase the oil recovery for horizontal and narrow fractures compared to vertical and larger fracture widths respectively.

van Wunnik and Kit [41] presented an analytical solution for steam injection into a fractured reservoir in which gravity drainage is the main mechanism of the oil production. They first gave an evaluation of the mixing rate and the steam/gas mixing zone in fracture networks. Using the temperature distribution in the reservoir and overburden rock, they derived the oil production rate by the mechanisms of gravity drainage and oil expansion.

Chen et al. [36] developed a dual porosity model for the simulation of thermal effects in naturally fractured reservoirs. Their simulator was 3-D, three-phase, and compositional. Matrix blocks were sub-divided into 2-D grids in order to consider effects of gravity, capillary pressure, and mass and energy transfer between fractures and matrix blocks.

Finally, Lee and Tan [38] introduced a multi-porosity/multi-permeability thermal simulator. They presented an iterative solution technique to create connection between any pair of blocks.

Boberg [42] discussed various mechanisms involved during the steamflooding of homogeneous reservoirs. A combination of mobility ratio improvement at the elevated temperature of the steam and a condensing gas drive displacement by the steam itself were mentioned as primarily mechanisms. Cracking of the oil at elevated temperatures, thermal expansion of the oil, solvent extraction, and temperature effects on the relative permeability to oil and water in the water zone ahead of the steam front are other mechanisms in steamflooding. He attributed the reason to a very low residual oil saturation after steamflooding in that hundreds of pore volumes of steam vapor travel through steam zone to the condensation front.

Willman et al. [43] examined the importance of the distillation of the light hydrocarbons during steamflooding in non-fractured cores. For a 50% distillable oil, they found up to 19.5 percent additional recovery due to distillation. The displacement efficiency of steam was also compared with that of hot and cold water. For the crude oil under investigation, the recovery for steamflooding was over 90% while under hot-waterfloods and cold-waterfloods they were around 70% and 60%, respectively.

Unlike homogeneous reservoirs, the injected steam does not sweep the porous media in fractured systems but preferentially flow through high conductivity fractures. Therefore, the above recovery mechanisms act differently in fractured systems. Reis [44] reviewed oil recovery mechanisms in fractured reservoirs during steam injection. Thermal expansion and gas generation were described as two key mechanisms at high temperatures. He also described several other mechanisms as follows:

Thermal Expansion: Fluid and rock minerals expand by increasing temperature. Since the expansion of matrix minerals reduces the porosity, a differential thermal expansion of the order of $0.05\%/^{\circ}\text{F}$ is created by the combination of porosity reduction and fluid expansion. These effects result in the expulsion of fluids from the matrix into the fracture. In addition, the mechanism of heating in fractured reservoirs is mostly by conduction, while in a homogeneous system heat is transferred mainly by convection through the condensation

of steam.

Capillary Imbibition: For water-wet reservoirs, capillary imbibition forces water in the fracture network into the matrix block through the smallest pores. Capillary imbibition, which depends on the brine/oil/rock system, may increase or decrease with temperature depending on the oil composition.

Gravity Drainage: Gas and water also transfer from fractures into surrounding matrix by gravity forces. The differential hydrostatic head between water in the fracture and a 35° API oil is only 0.065 psi/ft, while it is of the order of 0.3 psi/ft for gas in the fracture. Therefore, gravity drainage will have high potential recovery mechanism in gas filled fractures and thick formations.

Gas Generation: During steam injection, CO₂ generation was observed [39]. Light hydrocarbon components can also be generated during steam injection. As the temperature of reservoir increases, the volume of the generated gas also increases and displaces oil from the matrix towards the fracture. The distillation of light components at steam temperature is not significant in fractured system because the matrix blocks are not swept by the steam.

Solution Gas-Drive: Solution gas-drive can occur if the two phase envelope of a crude oil intersect the saturated steam curve. Reis [44] mentioned that in reservoir containing an initial gas saturation, this gas would expand upon heating and behave similar to a reservoir with an active solution gas-drive.

Some other mechanisms were also discussed by Reis [44], including chemical alteration of oil, cyclic pressure depletion, in-situ steam generation, alteration of the rock matrix, oil generation and rock compaction.

2.1.2 Flow Visualization Techniques

Flow visualization is a valuable device that enables us to understand some of the complex pore level mechanisms of multiphase flow in porous media, can confirm theories and upgrade computer simulation. Substantial efforts have been undertaken not only to visualize fluid flow during immiscible displacements [45, 46], but also for solution gas-drive [47], gravity drainage [48], and EOR processes, such as foam flow [49], surfactant and polymer flooding [50]. Although observing fluid flow in a single capillary tube or doublets is very useful, especially for the study of wetting phenomena [51], these tools are too simple to mimic the complex structure of capillary channels in real porous media. Therefore, investigators have been continuously searching for models with closer similarity to porous media. Typically, they make use of transparent Hele-Shaw cells, glass bead packs or micromodels. Persoff et al. [52] used 2 transparent rough-walled surfaces to simulate a single fracture. The history of the fabrication of etched glass and resin micromodels has been reviewed by Buckley [53]. In spite of the fact that such micromodels are restricted to two dimensions, they have been

very useful in understanding the complex relationship between the geometry and topology of the medium and the solid/fluid interactions [54, 55, 56, 57]. Recently, Hornbrook et al. [58] developed a new procedure to construct a high resolution replica of a porous medium. They transferred a digital image of a thin section onto a silicon wafer. The silicon wafer can be oxidized to obtain sandstone wettability and subsequently it is anodically bonded to a flat glass instead of fusion in the traditional glass-etched micromodel. The Appendix reports on the methodology used for the fabrication of a 2-D glass etched micromodel.

The majority of investigations so far was limited to replica of porous media. To our knowledge a systematic study has not been undertaken for network patterns having fractures along or across the flow direction to study effects of high permeability avenues in the fluid distribution during displacement. As a result, we do not have sufficient knowledge regarding the true mechanisms of drainage and capillary imbibition for oil recovery in fractured reservoirs. Furthermore, the role of fracture in fluid distribution and the relationship between fluid/solid interactions and flow parameters are ripe subjects for visualization investigations.

2.2 Steam injection in Matrix-Fracture Micromodels

In the previous chapters, we studied drainage and imbibition processes under fractured systems in isothermal conditions. Steam injection experiments in Hele-Shaw cells were also described to study the flow mechanisms in a geometry resembling a planar fracture. Some aspects of three-phase, two-component flow were demonstrated using a micromodel with dead-end pores. In this chapter, we complete the investigation by visualization of the flow mechanisms during steam injection in a glass micromodel mimicking the geometry of a matrix-fracture system. We, first, focused on the mechanisms originating from elevated temperature by uniform heating of the model without any fluid injection. Then, the injection of hot water was studied to investigate effects of an elevated temperature in the absence of phase change. Finally, different steam injection was carried out at different capillary numbers. Our observations were analyzed using the previous findings.

2.2.1 Experiments

The experimental set-up is basically the same as that for the isothermal displacement experiments. In addition, a steam generator consisting of a stainless steel tubing with $\frac{1}{16}$ inch diameter was used. A heater tape with two layers of glass wool were wrapped around the tubing, cold water being pumped into the hot tubing through a check valve using a syringe pump. The syringes for steam generator were of the gas-tight high performance type (Hamilton). The steam temperature was measured and controlled at the entrance of the model by a digital thermocouple temperature controller (Cole-Parmer). The temperature at different parts of the micromodel is measured periodically by a surface probe type T thermocouple. Due to very low steam rate, a high rate of heat loss, consequently a very fast condensation, were experienced. To avoid this, in some experiments we used additional insulation by placing two pieces of glass separated by a rubber spacer on both sides of the micromodel. In

some other experiments the model temperature was uniformly raised to decrease the heat losses. The following experiments were undertaken:

1. Heating of a model saturated with crude oil.
2. Hot water displacing crude oil or Dutrex 2621
3. Steam displacing mineral oil or Dutrex 2621.
4. Steam displacing crude oil.

In all experiments, the system was initially saturated with water. Injection of water or oil was done at conditions of secondary imbibition.

Heating of a Model Saturated with Crude Oil

The mechanisms originating strictly from rising the temperature of the model were investigated by the heating of a model saturated with oil, while both outlets were open to the atmosphere. We, first used a California type crude (viscosity 7000 *cP* at room temperature) in the triangular micromodel. By placing the model on a heater tape, the temperature of the model was slowly increased. Up to 45°C, a small amount of oil production was noticed. Oil expansion was responsible for this small production. At about 50°C, a gaseous phase started to develop (Fig. 12), originating from light components which vaporize. The bubbles nucleated in the micromodel at random places. These bubbles then started to grow towards the fracture (which has lower capillary pressure) (Fig. 13). The process of bubble nucleation and bubble growth have been recently studied by Li [56] in pressure depletion processes and by Satik [59] in boiling processes in porous media. Fig. 14 shows typical ramified shapes of bubble growth and the direction of growth towards the fracture. Fig. 15 shows that most of the crude oil is recovered only by this thermally-induced solution-gas drive at 50°C. Pentane with boiling point of 36.3°C, and hexane with boiling point of 69°C, are examples of light components that may exist and vaporize in crude oil. In order to measure the amount of these light components in our crude sample, we proceeded with a distillation experiment at low temperatures. Only about one percent by volume was collected at 50°C. At that temperature, we also noticed a small amount of non-condensable gas which evolved. In spite of the small amount of light components and dissolved gas, their effects on oil displacement were high due to the sharp contrast in densities between liquid and vapor, which exceeds a ratio of 1000. Thus, 1 percent of pentane in the liquid phase occupies more than 10 pore volumes in gas phase in our model. The associated production was, therefore, significant. In this process, the oil production continued even after gas breakthrough. At this stage, the vaporization involved a large number of snap-off events in the network (Fig. 16) with lamella created and stabilized by existing natural surfactants in the crude. Due to these snap-off events, much was drained along the roughness of the network.

We should point out that this mechanism was *not* observed during the same experiment involving Dutrex. In the latter case of Dutrex, which is a synthetic oil, no gas phase was observed until the temperature reached around 90°C. At this temperature, full evaporation started, and in a very short time, all the oil was completely recovered.

Figure 12: Bubbles nucleation during uniform heating of crude oil.

These experiments show that solution-gas drive process in natural light to medium crudes which contain amounts of light hydrocarbons can be very important mechanisms during steam displacement.

Injection of Hot Water

The injection of hot water to displace crude oil or Dutrex, was next carried out in order to study the effect of steam temperature alone without possible phase change or inertia effects. Hot water was injected at 97°C at three different capillary numbers. First, a set of experiments with Bakersfield crude oil in the triangular micromodel were undertaken. The model was initially heated to 40°C to reduce heat loss (but to prevent any vaporization). At the capillary number of 8×10^{-6} , it was observed that the hot water moved into the fracture first. The fracture was then blocked by a series of relatively stable lamellae. Because of this blockage of the fracture, water is forced to move into the matrix. Fig. 17 shows typical lamellae present in the fracture. When the lamellae created were broken by stretching in the fracture, further water penetration into the matrix was arrested. By the development of new bubbles in the fracture, water started again to invade the matrix. This process continued until all the network were penetrated (Fig. 18). Significantly, no foam was created in the matrix. This is in agreement with the theory of foam flow in heterogeneous media, which offers that foam is created in high permeability zones and forces displacements in low permeability areas. We reiterate that the creation of foam by hot water in the fracture is due to the development of a gas phase in the crude oil at high temperature and the existence

Figure 13: Bubble growth during uniform heating of crude oil.

Figure 14: Oil displacement during uniform heating of the model (snapshot 1).

! of natural surfactants in the crude.

Similar experiments were also carried out with Dutrex as well. Since Dutrex is a synthetic oil, the above components necessary for foam creation are not available; any lamellae created were easily broken.

Subsequent experiments with crude oil continued at the other two capillary numbers, 2×10^{-5} and 4×10^{-5} . Under these conditions, we also observed foam development. However, the lamellae were less stable, because of rate effects which cause lamellae to break more easily than in the case with lower capillary number. It will be seen in the following sections that in the case of steam injection, the high velocity of steam also makes the lamellae to break faster.

Hot water injection was also experimented with the square pattern micromodel. Both crude oil and Dutrex were tested. Here, the fracture was etched twice that in the matrix, and the fracture-to-matrix permeability ratio in this micromodel is much greater than in the triangular. The lamellae resulting from hot water injection were found to be less stable.

Steam Injection

This set of experiments was carried out to examine the application of steam injection, which was the ultimate objective of this dissertation. In this regard, we first carried out preliminary tests with mineral oil and Dutrex, then, a systematic set of experiments with crude oil at different capillary numbers was undertaken.

Steam-Mineral Oil Displacement

Figure 15: Oil displacement during the heating of the model (snapshot 2).

Figure 16: Snap-off after gas breakthrough.

Figure 17: Lamellae in the fracture result from hot water-crude oil displacement.

Figure 18: Hot water-crude oil displacement at $Ca = 8 \times 10^{-6}$.

In steam displacing mineral oil of a viscosity of 100 *cP*, the triangular pattern micromodel was used. The capillary number based on the equivalent water volumetric rate (0.108 *cc/min*) was estimated at 8×10^{-6} . The capillary number based on the steam velocity is also the same order of magnitude. Injected steam condensed at the beginning of the injection into the model, the resulting condensed water moving along the fracture first and subsequently penetrating into the matrix. In forced imbibition, the critical capillary number at which the displacement front in the fracture is ahead of the displacement front in the matrix is 5×10^{-6} , which is lower than the capillary number in the experiment. After the area around the inlet of the model became heated, steam started invading the matrix and displaced the remaining trapped oil. Since steam is non-wetting and of a low viscosity, a high velocity is required in order to reach the critical capillary number for the start of invasion of the matrix during drainage. Since we did observe matrix invasion, it can be concluded that the capillary number based on steam velocity is higher than the critical capillary number. The steam front in the fracture, however, is always ahead of that in the matrix (Fig. 19). In areas invaded by steam, due to the traveling of a large volume of steam vapor, and probably lowered interfacial tension at steam temperature, there was virtually no oil trapped. The oil displaced by steam injection moved towards the fracture in the form of an emulsion, while the steam front has the pulsation mechanism similar to what occurred in the Hele-Shaw cell [60], due to the condensation and subsequent restoration. Fig. 20 shows a magnified view of the condensation process in the fracture. After the model became heated, condensation

Figure 19: Steam displacing mineral oil

was relatively slow, and the steam front could be visualized for a few seconds. All these observations were also obtained in the experiment with kerosene which has a viscosity of 1.5 *cP* at room temperature. For both mineral oil and kerosene experiments, no foam generation was observed. The preliminary experiments above show how steam injection in a fractured system involves both drainage and imbibition processes.

Steam-Dutrex Displacement

In this set of experiments, we concentrate on the pore level mechanisms of steam displacement and the role of different fracture configurations. The micromodel in this experiment consisted of a square network adjacent to which are two fractures, one at the inlet perpendicular to flow direction, and another along the flow direction. Steam was introduced through the entire inlet by three paths etched in the micromodel from the injection port. The model was prewet. The capillary number based on equivalent water velocity was 8×10^{-6} . Due to the two-dimensionality of the model, there was a lack of communication between the condensed displacing water and the water film previously residing at the walls and corners of the network. Thus, condensed water first invaded the oil by meniscus movement only (Fig. 21). Then, it came into contact with preexisting water at the wall and displaced the oil. Fig. 22 shows water droplets in oil, which originated from the first contact of steam with the oil in fracture. Black areas in Fig. 23 show emulsions along the sides of the fracture.

Figures 24 and 25 show two snapshots of the experiment of steam displacing Dutrex. At the start of the experiment, steam moved through both fractures (Fig. 24). Later, steam penetrated into matrix network mostly from the inlet fracture rather than from the fracture

Figure 20: Close-up of steam in the fracture.

Figure 21: Close-up of condensed water invading oil by meniscus displacement.

along the flow direction (Fig. 25). This appeared to occur because of the high pressure drop near the inlet.

Fig. 26 shows an experiment of steam displacing Dutrex when the model was preheated to 50° C. In this experiment, condensation of steam is much slower and the steam front is much more stable (at 50° C, the viscosity of Dutrex is decreased substantially and the resulting pressure drop is lowered). Additionally, less heat loss due to a higher surrounding temperature produced less condensation.

Steam-Crude Oil Displacement

After these preliminary experiments, a parametric study of a steam-crude oil displacement at three different capillary numbers was undertaken. In this set of experiments, the micromodel with the triangular network was used. We employed a heavy crude sample from California with viscosity of about 7000 cP at room temperature. Steam was injected at three different rates with corresponding capillary numbers of 8×10^{-6} , 2×10^{-5} , and 4×10^{-5} . The capillary numbers were calculated based on an equivalent cold water velocity. In order to be able to compare steam-flooding with water-flooding under similar conditions, we also injected cold water at the same capillary numbers as above. In all experiments either steam or water injection, the crude was initially maintained at the temperature of 40°C. This preheating was necessary to decrease heat losses during steam injection. (Higher temperatures were not tried since at temperatures around 45°C, a gaseous phase from the light components of crude or dissolved gas started to develop).

Figure 22: Close-up of water-in-oil emulsion.

Figure 23: Emulsion along the sides of the fracture.

Figure 24: Steam displacing Dutrex (snapshot 1).

Figure 25: Steam displacing Dutrex (snapshot 2).

Figure 26: Steam displacing Dutrex (preheating at 50° C).

Steam injection at $Ca = 8 \times 10^{-6}$: The first steam injection experiments started with the rate of 0.108 cc/min of equivalent cold water which corresponds to $Ca = 8 \times 10^{-6}$. The model was preheated at 40°C. At this temperature bubbles did not nucleate. Since the steam rate was low, and due to the initial presence of oil in the fracture, the steam condensed right at the inlet. The condensed water moved first through the fracture, with only a few pores penetrated in the matrix. We reason that this occurred because the rate of water is higher than the critical rate for imbibition, in which the displacement front in the fracture is ahead of the displacement front in the matrix. Also, the corresponding capillary number is barely higher than the critical capillary number for drainage. A drainage process may be applicable if we assume that the water is non-wetting due to the lack of communication with the connate water in a 2-D model when a heavy oil is present. In either case the capillary number does not suffice for a considerable penetration in the matrix. After steam injection continued, additional condensed water penetrated in the matrix (Fig. 27). The reason for this is that at the steam temperature, gas bubbles evolved and temporarily blocked the fracture, resulting into a high pressure drop which led to a displacement towards the matrix. Fig. 28 shows snapshot of steam displacement. It is important to notice that steam moves through the fracture, with only a few pores invaded in the matrix. Fig. 29 shows a close-up of steam in the fracture. In spite of the fact that all oil around the fracture was completely displaced and there was not substantial pressure drop due to the presence of oil, steam moves preferentially through the fracture. We explain this by noting that steam is the non-wetting phase and at capillary number values below the critical for invasion of matrix in drainage,

Figure 27: Steam displacing crude oil at $Ca = 8 \times 10^{-6}$ (snapshot 1).

no penetration is expected to occur. Fig. 30 is another snapshot of the experiment in which most of the oil is displaced, while the steam front in the fracture has reached to about half of the model. In another experiment, cold water was injected to displace oil at the same conditions. Cold water similar to the condensed water did enter the fracture at the beginning of steam injection. After some time, a small area near the inlet was also penetrated with water (Fig. 31). By comparison of water-flooding and steam-flooding experiments, we can measure the efficiency of steam displacement in fracture systems. Thermally induced solution gas drive and viscosity reduction are the main mechanisms for the increased efficiency.

Steam injection at $Ca = 2 \times 10^{-5}$: Steam injection experiments were then conducted at the capillary number $Ca = 2 \times 10^{-5}$. The beginning of this experiment is similar to the previous. Condensed water enters the model and first displaces all oil in the fracture (Fig. 32). This is due to the fact that the corresponding capillary number is higher than the critical for either imbibition or drainage. After some steam injection, steam did penetrate the matrix. Fig. 33 shows that steam enters the matrix indicating that the critical capillary number condition is met. The steam fronts in the fracture and matrix are shown in Fig. 34, where the steam in the fracture is ahead of that in the matrix. We note that in those areas displaced by steam, there is no residual oil. Here, similar to the previous, a cold-water injection at the same conditions was also carried out. Now, a viscous finger was created in

Figure 28: Steam displacing crude oil at $Ca = 8 \times 10^{-6}$ (snapshot 2).

Figure 29: Close-up of steam in fracture during steam-crude oil displacement.

Figure 30: Steam displacing crude oil at $Ca = 8 \times 10^{-6}$ (snapshot 3).

Figure 31: Cold water displacing crude oil at $Ca = 8 \times 10^{-6}$.

Figure 32: Steam displacing crude oil at $Ca = 2 \times 10^{-5}$ (snapshot 1).

Figure 33: Steam displacing crude oil at $Ca = 2 \times 10^{-5}$ (snapshot 2).

the matrix in addition to the displacement in fracture (Fig. 35). Nonetheless, the difference between steam and cold water displacement efficiency is clear.

Steam injection at $Ca = 4 \times 10^{-5}$: Finally in the last experiment, the capillary number $Ca = 4 \times 10^{-5}$ was tested both for steam injection and cold water experiments. Figures 36 and 37 show two snapshots of steam injection, while Fig. 38 shows the cold water experiment. In Fig. 36, an early finger in the matrix is observed, as a result of the condensed water. Similar fingers were observed in the cold water experiment (Fig. 38). Since the capillary number is relatively high here, we did not detect any imbibition mechanism, but rather a displaced process involving meniscus movement detect. Therefore, Figures 36 and 38 are comparable to the displacement simulated in Fig. 2.15.

2.3 Conclusions

Pore-level and larger scale visualization of steam and hot water displacement, as well as thermally-induced solution gas drive in a micromodel mimicking a fractured system were carried out. Different oils at different capillary numbers were tested. Also, different configurations of the fracture were examined. In the steam displacement experiments, it was found that the steam enters into the fracture or the matrix depending on the steam rate. If the

Figure 34: Steam displacing crude oil at $Ca = 2 \times 10^{-5}$ (snapshot 3).

Figure 35: Cold water displacing crude oil at $Ca = 2 \times 10^{-5}$.

Figure 36: Steam displacing crude oil at $Ca = 4 \times 10^{-5}$ (snapshot 1).

Figure 37: Steam displacing crude oil at $Ca = 4 \times 10^{-5}$ (snapshot 2).

Figure 38: Water displacing crude oil at $Ca = 4 \times 10^{-5}$.

capillary number exceeds the critical, steam can displace the fluids in the matrix, otherwise it moves into the fracture only. This critical number corresponds to that previously discussed in the isothermal displacement of drainage. Forced imbibition during steam-flooding was also visualized. Whether the condensed water moves preferentially into the fracture or the matrix also depends on the other critical capillary number for imbibition, which was found to be a function of the geometric properties of the matrix and the viscosity ratio. At the pore level, it was shown that most of the oil trapped by condensed water can be mobilized and recovered when in contact with steam. A steam pulsation mechanism, due to the condensation and subsequent restoration, was evident. Evaporation of light components existing in crude oil or gas generation may induce a very high efficient gas drive mechanism. Viscosity reduction and oil expansion were observed, as two important effects when steam displaces highly viscous oil. Natural surfactants existing in the crude oil in conjunction with gas generation at high temperatures can lead to the formation of stable lamellae in the fracture and to an improved displacement in the matrix. In general, we found that steam displacement in fractured systems can be an efficient EOR process.

3 A Pore Network Model for Foam Formation and Propagation in Porous Media

Hooshang Kharabaf and Y. C. Yortsos

3.1 Introduction and Literature Review

The successful application of foam in EOR requires efficient numerical models in addition to theoretical postulates and experimental information on the flow behavior at reservoir conditions. During foam injection in oil reservoirs, the transient behavior is certainly the most dominant stage of the process. Therefore, both experimental data and foam flow theories on this particular stage are needed to establish accurate field scale numerical models.

Investigators working on different aspects, proposed various patterns for the foam flow. Mahmood and Brigham [61] summarized the behavior observed to seven types: (1) Bubble flow, (2) Intermittent flow, (3) Plug flow, (4) Trapped-Gas flow, (5) Segregated flow, (6) Membrane flow, and (7) Tubular-Channel flow. The many different regimes and the apparent disagreement among the various investigators show the necessity of rigorous microscopic studies concerning the foam flow mechanisms.

In fluid flows in porous media, the simulation of the process at the pore level is very important. Typical reservoir simulators consider the flow in an "averaged" Darcy-scale medium. However, simulations at the pore-scale level can reveal many important aspects of the complexity of foam flow in porous media. At present, pore-network models of foam generation and propagation are rare in the literature. Models dealing with foam flow simulation are usually static, using classical percolation concepts [62, 63, 64, 65, 66], which are applied inappropriately.

The conditions for governing generation and propagation of lamellae in porous media are still a controversial issue in the study of foam flow. Ransohoff and Radke [67] reported the existence of a minimum flow rate for foam generation. According to their results, strong foams were formed only above a critical capillary number. The corresponding critical velocity is very high and not practical for field conditions. Rossen and Gauglitz [65] derived equations for finding a minimum pressure gradient $|\nabla P|^{min}$, for both continuous and discontinuous gas regimes, by employing percolation theory and using the fact that a minimum pressure gradient is needed to displace lamellae out of a pore throat. Their conclusion was similar to the critical velocity criterion (minimum velocity requirement) that was already discussed.

Chou [62] presented a statistical network model using percolation theory to show that foam generation mainly depends on the pore size distribution. According to his model, lamellae are stationary at pore throats, but they may break and remake. He believes that there is no minimum pressure gradient requirement to generate or to propagate foam in porous media. On the contrary, Rossen and Gauglitz [65] believe that there is a minimum pressure gradient requirement to mobilize foam in porous media. He also used a percolation approach to calculate the minimum pressure gradient, and other parameters of the system.

Miller and Fogler [64] studied the formation of conductive pathways and the accompanying permeability increase with increasing pressure and inducing individual lens rupture. In their work, the fractal dimension of the first conductive channel ranges from 1.89 to 1.06 for high and low elastic modulus gels, respectively. They believe that the dependence of percolation and breakdown in their work is unique and produces an enormous range of breakdown behavior for any degree of microscopic heterogeneity. The key mechanism included in their model, in comparison to other similar models, is the accounting for the elastic deformation of gelled lenses at pore throats, which appear to affect the distribution of the pressure in the gas and subsequently the stress field in other lenses. The "fractal dimensions" obtained in their work are subject to uncertainty, because of the small lattice sizes reported.

Laidlaw *et al.* [63] report the results of a pore-scale investigation of mechanisms for the alteration of mobility by foam lamella blockage in a porous medium. Saturation and relative permeability curves were obtained using well-known power-law expressions of percolation theory. The qualitatively different features of gas mobility by foam claimed can be described using two adjustable parameters that characterize the throat size at which blockage commences, and the degree of blockage. This model is similar to the model presented by Rossen and Gauglitz [65], in considering continuous gas pathways near the percolation threshold. The effect of foam is to block an infinite conducting cluster, initially well above the percolation threshold, until the percolation probability, p , moves near the percolation threshold, p_c . This will result into a change in the relative permeability of the gas, the saturation of continuous gas phase, and the gas mobility of the medium.

Other works dealing with pore-scale study of foam and related issues also considered a classical percolation concept at their analysis [68, 66]. None of the above mentioned works, however, simulates a *dynamic* invasion process. As a result, the preferential invasion of low permeability layers by blocking high permeability layers was never observed. The minimum pressure gradient path (minimum threshold path) was never determined and the properties of the path was often inappropriately approximated by the "chemical distance", which is the shortest path between two points in an infinite percolation cluster. With the exception of Rossen and Mamun [68], the effect of throat-size (threshold) distribution on the minimum pressure gradient value and the minimum threshold path, was never addressed. Even these authors, however, believed that shifting the probability distribution function of the thresholds will only shift the minimum pressure gradient accordingly, without changing the properties of the path as well. All these misinterpretations arise from an ill-misanalogy between this process and classical invasion percolation.

Laboratory data for the transient displacements during foam injection are few. Baghdikian and Handy [69] studied the transient behavior of simultaneous flow of gas and surfactant solution in consolidated porous media. Several of the factors that contribute to the foam generation were described. A systematic study of foaming with different fluid velocities and foam qualities provided extensive data for foam flow conditions. Two foam flow regimes, "weak" and "strong" foam were identified. Results indicated that in some cases, an excessively large number of pore volumes of foam injection is necessary to propagate foam deep into the reservoir (see Ref. [69]). These corresponded to lower gas and surfactant velocities,

where foam generation was not expected according to the critical gas velocity criterion cited before [67]. Higher gas injection velocities reduced this foam "incubation time" in their experiments. Many of their observations, however, cannot be explained by existing theories.

In this section, a pore-network model of foam formation and propagation, is introduced for the first time. The model simulates a *dynamic invasion* process, in which gas invades porous medium occupied by a surfactant solution. During the invasion, lamellae by leave-behind and snap-off mechanisms are generated. The latter mechanism may block the continuous gas pathways. In case the gas phase remains continuous, the pressure difference necessary for the front advance, is the minimum capillary pressure needed at the gas front. If the gas phase becomes discontinuous, the *overall* pressure difference between the two phases to mobilize the gas and force the invasion at the front, needs to be higher than a certain amount. This pressure difference for discontinuous cases, is the sum of two types of pressure differences in the system: The local capillary pressure at the gas front as in the continuous case, and the pressure difference necessary to mobilize a series of lamellae in the blocked gas pathway, to push the gas at the front. Obviously, according to this mechanism, at any time, a path requiring the minimum overall pressure difference needs to be identified, and mobilized. Using a novel algorithm, the path at any stage of the displacement was determined. From this, the fraction of the flowing lamellae in the system, $\mathcal{X}_f$, the fraction of the trapped lamellae, $\mathcal{X}_t$, the gas phase saturation, S_g , and the minimum pressure gradient, $|\nabla P|^{min}$, are calculated. It is found that, in the case of transient displacement, $\mathcal{X}_f \rightarrow 0$.

A further increase in the pressure difference, could cause more than one gas path to open and conduct. This mobilization process is studied by using a more elaborate algorithm. Employing such a simulator, the pressure gradient to mobilize even the last lamella in the system can be determined, and the corresponding $\mathcal{X}_f$, $\mathcal{X}_t$ and S_g at any applied pressure gradient can also be computed.

The main controlling parameter in this model is the "snap-off probability" for a lamella. The model allows for various parameters or processes, currently empirically treated in previous models, to be quantified and interpreted. The sweep efficiency of the system for disordered homogeneous and heterogeneous media at *strong* or *weak* foam conditions are calculated. Finally, history and profile plots for pressure difference, gas saturation, snap-off and overall lamella density of the system at different pore volumes of injection and at various locations are provided. Comparison of these results with experimental and reservoir-type simulation results is shown to be in quite a good agreement.

3.2 Model and Assumptions

A porous medium is a two-phase material, consisting from solid matrix and interconnected voids (pores). Two important features of a natural porous media are the irregularity of shape and the variety of the pore sizes. The study of flow in porous media depends greatly on the geometry, topology and size distributions of pore bodies and pore throats.

In this work, the porous medium is simulated by two- and three-dimensional lattices, having coordination numbers 4 and 6 (for simplicity), and bonds and nodes representing

Figure 39: Drainage displacement, film deposition and snap-off of a wetting liquid in a constricted cylindrical pore (from Ref. [28]).

pore throats and pore bodies, respectively. For size distribution of either throats or sites any arbitrary probability distribution function can be used. Here, a Rayleigh distribution of pore throat sizes

$$\alpha_t(r) = \frac{\pi r}{2\bar{r}_t^2} \exp\left[-\frac{\pi r^2}{4\bar{r}_t^2}\right] \quad (18)$$

with average radius ($\bar{r}_t$) is used. Pore body sizes may also be distributed using known correlated techniques [70, 71, 72]. The reason of having both distributions, would be to control the site-bond size ratio (aspect ratio), which in turn controls the snap-off mechanism in the system. In other words, the distribution of the pore sites and the amount of overlap between the two distributions, along with the critical aspect ratio, dictates the probability for snap-off mechanism. We call this the *snap-off probability*, f_{so} . We will use this parameter instead of worrying about the pore size distribution, the overlap of the two distributions, or the critical aspect ratio of the system.

We consider the case in which, flow injection and flow drainage takes place from two opposite sides of the network. In all other sides, periodic boundaries are enforced to reduce boundary effects of the network.

The system is initially occupied by a liquid phase, such as a surfactant solution. By injecting gas from one end, this liquid is displaced. As the pressure in the non-wetting phase increases gradually and the gas displaces the surfactant solution, the model allows for lamellae generation. From the described three mechanisms for lamellae generation, only snap-off and leave-behind mechanisms will be included in the model.

Snap-off is the result of an instability due to the curvature difference between pore throats and pore bodies. Assuming uniform pressure over the gas phase, this provides a higher

capillary pressure (lower liquid pressure) at the pore throats. Thus, via solid corners, more liquid is withdrawn towards the throat and eventually a liquid film at the location generates (Figure 39). For this mechanism to occur, the pore body to pore throat size ratio (*aspect ratio*) needs to be higher than a critical value, believed to be between 1.5-2.5 [73, 74, 75, 76]. Snap-off is possible during both drainage and imbibition, no matter whether surfactant exists or not. The role of surfactant is to stabilize unstable thin liquid films.

Leave-behind mechanism is assumed to be possible whenever bond trapping is permitted in the wetting phase. As the pressure difference between two phases increase, the trapped liquid at the pore throats drain and lenses are generated. In case there is surfactant present in the liquid phase, an increase in the gas phase pressure causes lenses to thin and to create lamellae.

For a non-wetting phase to displace a wetting phase, a pressure drop P_c across the interface must be exceeded. For a cylindrical throat of radius r_F at the front, after neglecting gravitational forces, this capillary pressure is

$$P_c = \frac{2\gamma}{r_F} \cos\theta, \quad (19)$$

where θ is the contact angle, which depends on the fluids, type of rock, and roughness of the surface. We will take for simplicity $\theta = 0$, and estimate r_F , by its smallest value $r_{F,t}$ (at the pore throat), thus,

$$P_c = \frac{2\gamma}{r_{F,t}}. \quad (20)$$

In case there are sufficient lamellae generated by snap-off, the gas phase can become discontinuous. Continuing the displacement in such a case would require first, mobilizing some train of lamellae in a path. For this, the pressure difference across each lamella, i , needs to be higher than $4\gamma/r_{min,i}$ [65], where γ is the interfacial tension between wetting and non-wetting phases and $r_{min,i}$ is considered to be equal to the pore throat radius, ($r_{t,i}$). For a single lamella, this is almost twice the pressure difference between the invading and defending phases during capillary invasion of the same throat size. Obviously, capillary forces are very small compared to the yield stress-type forces necessary to mobilize a series of lamellae in one path, $\Delta P_{yld} = \sum_i 4\gamma/r_{t,i}$. Here, the summation is taken over any blocking lamellae, i , in a single path. Accordingly, it would be a good assumption to neglect viscous and gravitational forces which are only comparable with capillary forces. However, these forces will become important when f_{so} is small and capillary forces dominate. We should notice that capillary forces are not neglected here.

By increasing the pressure of the injected phase and before the next invasion can take place, one or more of the lamella(e) (generated by either mechanism) must be mobilized. In such a case, it is possible that stretching will cause a lamella to rupture when it moves out of the pore throat and reaches the next pore body. Here, it will be assumed that another lamella will rapidly snap-off at the same throat location, thus, the pressure difference in the trapped gas phase remains relatively unchanged. In addition, by assuming incompressible gas flow, for simplicity, the overall pressure difference increase in the system will act to

displace the train of lamellae in any path. If the pressure difference increase is sufficient, the path with the minimum overall resistance will be mobilized and invasion at the front will take place. This process will continue until foam breaks through.

The model also allows for trapping in the liquid phase. Trapping is a mechanism which must be considered during, whenever flow in the roughness is negligible. Under such condition, part of the wetting phase (which become surrounded by non-wetting phase) cannot escape or be swept and remains in place.

3.3 Simulation and Results

The following steps are considered by the simulator during the displacement process:

1. Using at any stage an algorithm similar to the one described in [77], we can identify the path with the “minimum overall pressure potential” in gas invaded phase. We consider the minimization of $\Delta P_{ov}^{min} = P_c + \Delta P_{yld}$ over all possible paths in the invaded phase.
2. By increasing the pressure difference between the two phases, to the new value ΔP_{ov}^{min} , gas invades the newly accessible pore throats and the following pore sites at the front. This is done only one site-at-a-time (similar to a constant flow rate invasion).
3. With a probability equal to or higher than f_{so} , the newly invaded pore throat may snap-off. If so, a lamella generates at the pore throat.
4. Occupied pore sites may generate leave-behind lamellae with $Z - 2$ neighboring sites, where Z is the lattice coordination number. The code identifies such possibilities and, if necessary, generates leave-behind lamella(e).
5. The trapping of the liquid phase in the invaded zone is checked, and trapped sites are prevented from being potential invading sites in the following steps.
6. If there are additional pore sites for further invasion, the process is repeated.

The initial condition for the simulation is that the porous medium is fully occupied by a surfactant solution. As mentioned earlier, in all sides of the network other than the inlet and outlet, periodic boundaries are considered.

3.3.1 Transient Displacement

Displacement Patterns

We first show different snapshots of foam displacement in a 2- D lattice. Figure 40 illustrates foam invasion in a 200×200 lattice at two different stages, where the front has advanced to $0.5L$ (Fig. 40a), and at breakthrough (Fig 40b). L is the lattice size in the flow direction. The snap-off probability, f_{so} , in this case is maximum and equal to 1. This means that all invaded throats in the system will snap-off, and the simulator will generate a *strong* foam. The result is a very compact invaded zone, where almost all the liquid has

Figure 40: Foam displacement in a 200×200 lattice, for $f_{so} = 1$. The grey area shows the invading phase, the dark area shows non-invaded phase. Trapped sites in the invaded zone are also denoted by dark color. The path shown is the minimum overall pressure potential path at: (a) $x_F = 0.5$, and (b) $x_F = 1$.

been swept, which is characteristic of a strong foam. In the figure, dark area represents the initially liquid-occupied zone, the grey area shows the foam invaded zone. Dark small areas inside the swept zone are liquid trapped areas, which in this case includes a very small fraction of the invaded section. This shows that for such a strong foam, sweep efficiency is very high. At each particular snapshot, the black path in the invaded area shows the minimum overall pressure potential path. These paths are similar to the *MTP* discussed in [77]. Notice that here, instead of using a uniform distribution of thresholds, a Rayleigh distribution for throat radii are used. However, invaded patterns and the minimum pressure gradient paths are similar to the *IPM* process. Another difference between the above and the *IPM* process is that, here, the resistance at the front before ($2\gamma/r_F$) and after ($4\gamma/r_F$) advance is different, whereas in the *IPM* process it remains the same (equal to the threshold resistance).

Figures 41(a-c) correspond to foam displacement in a 100×100 lattices with f_{so} equal to 0.7, 0.5 and 0.35, respectively. As the snap-off probability parameter, f_{so} , decreases, giving a smaller chance for snap-off lamellae generation, fewer lamellae block the continuous gas pathways. As a result, both the front and the minimum pressure gradient paths become more tortuous, and larger areas of liquid become trapped. It can be easily seen that the sweep efficiency decreases as the snap-off probability parameter becomes smaller. This shows the importance of the snap-off mechanism. For small f_{so} , even though the leave-behind lamellae are still being generated with the previous probability, the leave-behind lamellae do not play major role in changing the sweep patterns of displacement, whereas the snap-off lamellae are still those which block the continuous gas pathways. If the gas pathways do not become blocked, the gas pressure will be the same over all the swept zone, and as a result the capillary forces will be the only forces dominating at the invading gas front, because viscous forces are neglected. In such a case, the process will become identical to invasion percolation.

Invasion percolation model, was first proposed by Chandler *et al.* [78] and, Wilkinson and Willemsen [79] to describe capillary controlled fluid flow in a porous medium. Figure 42 shows a displacement process for $f_{so} = 0$ in a 200×200 lattice. The pattern is similar to invasion percolation cluster. The front, the invaded cluster and the minimum pressure gradient path are all self-similar. The minimum pressure gradient path is the backbone of a mixed bond-site percolation process. The properties of this type of invasion process has been discussed in [77].

As soon as the snap-off lamellae become generated and block the continuous gas phase, yield stress type of forces of lamellae become remarkably dominant and control the invasion processes and the sweep efficiencies.

Sweep Efficiency at Breakthrough

Figure 43 shows the sweep efficiency, E_s , vs. snap-off probability, f_{so} , at breakthrough for different lattice sizes ranging from 50×50 to 200×200 in 2-*D* and from $15 \times 15 \times 15$ to $30 \times 30 \times 30$ in 3-*D*. It is interesting how fast the sweep efficiency increases as more snap-off lamellae become generated. Sweep efficiencies vary from about 30% for no snap-off to 97% in the full snap-off case. At $f_{so} = 1$, about 96% of the throats contain lamellae. Simulation results show that about half of these lamellae are generated by leave-behind and

Figure 41: Foam displacement in 100×100 lattices, where f_{so} is equal to (a) 0.7, (b) 0.5, and (c) 0.35. As f_{so} decreases, the minimum pressure gradient path and the advancing front become more tortuous, and more liquid becomes trapped.

Figure 42: Displacement in a 200×200 lattice, where $f_{so} = 0$ at (a) $x_F = 0.5$ and (b) $x_F = 1$. The process is identical to invasion percolation. Here, the minimum pressure gradient path is the backbone of a mixed bond-site percolation process. The liquid-trapped fraction is almost the same size as the invaded part.

Figure 43: Sweep efficiency at breakthrough vs. snap-off probability in 2-D lattices.

the other half by snap-off mechanisms. At $f_{so} = 0$, where the snap-off lamellae cannot be generated and the process is similar to invasion percolation process, only about 30% of the liquid-occupied pore sites are swept at breakthrough, even though about 8% of the overall throats in the system contain leave-behind lamellae. This means that for each two invaded pore sites in the system, there is at least one leave-behind lamella. But these lamellae do not block the gas pathways and the gas phase remains continuous. Their only role is to create a fully dendritic, loopeless infinite cluster of gas.

Our previous studies [80] show that in such cases, there is no minimum pressure gradient requirement for the onset of foam mobilization. The first lamella to be mobilized is always a leave-behind lamella. In these studies, a pore-network was employed to model the onset of foam mobilization in a continuous gas phase. In the model, liquid was first displaced using a drainage process, to a certain percolation probability, p' , well above the percolation threshold, p_c . Later, applying an imbibition rule at the throats, the system generated snap-off lamellae and moved percolation probability backwards to p_c , by closing smaller throats of the displaced cluster. This was continued to a certain p' above p_c , where the gas phase still remained continuous. Then, the simulator finds the minimum pressure gradient for mobilizing the first lamella and locates the corresponding lamella location. It was found that the very first lamella to be mobilized is always a leave-behind lamella, generated from the long dendrites created at the percolation threshold. In addition, it was found that the minimum pressure gradient to mobilize that particular lamella is inversely proportional to the lattice size. In other words, if one is going to mobilize the first lamella in a continuous gas phase generated by a classical invasion percolation model, the minimum pressure gradient for the onset of lamella mobilization (always leave-behind) will be zero for large network sizes. This idea was once again confirmed using our novel and more elaborate model. It is worth recalling that even pore-network model for classical invasion percolation was never tried.

Minimum Pressure Gradient for the Onset of Foam Mobilization

Figure 44(a,b) shows the minimum pressure gradient required for the onset of foam mobilization in 2- D and 3- D lattices, respectively, as the snap-off probability varies from 0 to 1. The difference between the strong foam in one extreme ($f_{so}=1$) and the weak foam in the other ($f_{so}=0$) is very significant. When there is no snap-off block in the system, the minimum pressure gradient is zero. We recall that even at $f_{so} = 0$, there are still many leave-behind lamellae in the system that could be mobilized. This is the case of a very weak foam. As the system starts to generate more and more snap-off lamellae, at some f_{so} , the gas phase becomes discontinuous. Following this, there is a minimum pressure gradient to mobilize the lamellae and let the gas to advance. From the limited data, it appears that there is a *critical* snap-off probability value, approximately equal to ~ 0.35 in 2- D , and ~ 0.65 in 3- D , where gas phase discontinuity begins. Even if more accurate values were found, it should be reminded that they would be only valid for that particular pore throat radii distribution. Nonetheless, it is expected that the trend will be similar for other distributions. Another interesting observation is that the normalized values of minimum pressure gradient at $f_{so} = 1$, for 2- and 3- D lattices seem to be fixed. A normalization has been considered

Figure 44: Normalized minimum pressure gradient *vs.* snap-off probability in (a) 2-*D*, (b) 3-*D* lattices.

to make the minimum pressure gradient equal to 1 for a straight lattice size path, where average throat radii are assigned to all bonds. So, for a given distribution $|\nabla P|^{min} \approx 0.98$ and $|\nabla P|^{min} \approx 0.85$, for 2-*D* and 3-*D* lattices, respectively.

There are some other points in these figures that need further discussion. First, the gas phase becomes discontinuous at snap-off probabilities higher in 3-*D* than in 2-*D*. Considering the topology of the lattices, this is reasonable and expected. Second, for a similar dimension as the lattice size increases, the critical snap-off probability for a non-zero minimum pressure gradient increases. This could be due to a finite lattice size effect, but it should not lead to the conclusion that the minimum pressure gradient becomes zero at larger systems. Because, Fig. 44 further shows that the $|\nabla P|^{min}$ is the same (if not greater) for larger lattices of the same dimensionality. This means that there is a fixed minimum pressure gradient for each dimension, and the value at $f_{so} = 1$ will not decrease. This is also expected, considering the system's behavior in these cases ($f_{so} = 1$), which is very similar to *IPM* processes. Again it needs to be pointed out that, these values cannot be generated from, neither are related to, classical invasion percolation. Only the newly introduced class of invasion processes can account for the yield stress forces during the dynamic invasion, and are capable of correctly predicting foam simulation results.

Figure 44 shows a very important characteristic of foam flow, the one which has been a matter of consideration and controversy for a long time. As mentioned in the introduction and literature reviews, many investigators believe that there is a minimum pressure gradient for the onset of foam flow in porous media, while others rejected this idea and claimed that foam can be generated even at small pressure gradients or low flow rates. Each group had experimental and analytical data to support their own idea. Even if sometimes inappropriate concepts of classical invasion percolation were used, the laboratory results cannot be wrong. Interestingly our simulation results confirm both groups' claims. In other words, we show that in generating weak foams no minimum pressure gradient is required for the onset of foam flow, but when the system is capable of generating (specially a very) strong foam, there is a minimum pressure gradient requirement. Because it is not possible in real systems, to define exactly a *very strong foam*, it is very difficult to come up with only one corresponding *universal* minimum pressure gradient value. As explained earlier, this value will also depend on many system parameters, such as the pore geometry and topology, and the chemical and physical properties of the rocks and surfactant solutions, relative permeabilities and the fractional flow of the fluids, *etc.*

It is believed that, the system's many internal factors play a more important role in generating a strong foam and consequently the minimum pressure gradient requirement for mobilization, than external factors, such as imposing a certain pressure gradient. And as the lamellae number density of a system is increased, the minimum pressure gradient may become involved and its value may correspondingly increase.

History and Profile Plots of Transient Displacement

Among the information needed during the transient foam flow displacement in porous media, is the history and the profile of quantities, such as pressure difference, foam saturation, and foam texture during the invasion process. Our simulator allows conveniently to obtain

such information of interest, at any pore volume of injection and from any system location. Figures 45 through 48 show the profiles of gas pressure difference, foam saturation, lamellae number density of snap-off, and of both mechanisms, respectively. The displacement is taking place in $30 \times 30 \times 30$ lattices. Each figure considers four different snap-off probabilities; (a) $f_{so} = 0$, (b) $f_{so} = 0.5$, (c) $f_{so} = 0.7$, and (d) $f_{so} = 1$, ranging from weak to strong foam. Either plot shows the profiles of the quantities at four different stages, where the very first front proceeds to the normalized front location at $x_F = 0.25, 0.5, 0.75$ and 1 , distinguished by different lines. The corresponding pore volumes of the gas injected are also provided.

Figure 45 shows ΔP_g profiles within the gas phase for different cases and at different stages. Here, ΔP_g is the normalized average pressure difference in the gas phase between every invaded location and the invading front. Therefore, it does not include the pressure difference between the gas and the liquid phase (capillary pressure) at the front. The average is taken among all pore sites at every fixed x . Different cases are considered. Figure 45a shows the case for $f_{so} = 0$. As the gas is being injected, ΔP_g remains zero. The reason is obvious, as the gas phase is a continuous phase (similar to invasion percolation cluster) and viscous forces are neglected. In case (b) where $f_{so} = 0.5$, snap-off lamellae are generated and the gas phase is partially blocked (see Fig. 45b). However, there are still some continuous paths in the system. These continuous paths result into having zero minimum pressure gradient requirement at the onset of foam flow, while trapped gas in the invaded phase causes having average pressure difference other than zero. The next case Fig. 45c, considers the higher snap-off probability of $f_{so} = 0.7$, above the discontinuity threshold. This time the snap-off probability is so high that the gas phase is completely discontinuous. In order for the front to advance, it is necessary that all of the lamellae and trapped gas (bubbles), residing in the minimum pressure gradient path, be mobilized. The corresponding ΔP_g of this system is higher than the previous case (b), even if the pore volume of gas injected (liquid swept) are close. The ΔP_g profiles of this case are more stable than the previous, showing that the invading front is becoming more stable. Finally Fig. 45d shows a case for $f_{so} = 1$. Here, all throats in the invaded gas contain lamellae, ΔP_g is much higher, and the pressure profiles in the system are very smooth, showing that the fronts are stable at various stages of invasion.

Figure 46 illustrates foam (gas) saturation profiles for the same cases and the gas front approaching the same locations. This figure qualitatively shows the effect of having strong foam in comparison to having weak foam. It is noticeable how the gas saturation in the system increases with increasing snap-off probability. Another point is that in weak foams (cases (a) and (b)), the foam front is unstable, and as shown earlier, the pattern is similar to a percolation cluster. Whereas, for strong foam, the invading phase becomes stable at the back and there are smooth and sharp transition zones at the front. This characteristic of the system becomes more relevant for case (d), where $f_{so} = 1$. In this case, three different regions of piston type displaced zone at the back, non-invaded initially liquid-occupied zone at the front, and a sharp transition zone in-between, are completely distinguished. In addition, this figure shows that the trapped liquid fraction is very high in weak foams, but it becomes very small in strong foam displacement.

Figure 45: Normalized gas pressure difference, ΔP_g , profiles at various snap-off probabilities; (a) $f_{so} = 0$, (b) $f_{so} = 0.5$, (c) $f_{so} = 0.7$, and (d) $f_{so} = 1$. Each figure shows four different stages, where the front approaches the normalized front location at $x_F = 0.25, 0.5, 0.75$, and 1. The corresponding pore volumes of the injected gas are also provided. Simulations are for $30 \times 30 \times 30$ lattices.

Figure 46: Gas saturation profiles at various snap-off probabilities; (a) $f_{so} = 0$, (b) $f_{so} = 0.5$, (c) $f_{so} = 0.7$, and (d) $f_{so} = 1$. Each figure shows four different stages, where the front approaches the normalized front location at $x_F = 0.25, 0.5, 0.75$, and 1. The corresponding pore volumes of the injected gas are also provided. Simulations are for $30 \times 30 \times 30$ lattices.

Figure 47: Snap-off lamellae number density, $\mathcal{N}_{so}$, profiles at various snap-off probabilities; (a) $f_{so} = 0$, (b) $f_{so} = 0.5$, (c) $f_{so} = 0.7$, and (d) $f_{so} = 1$. Each figure shows four different stages, where the front approaches the normalized front location at $x_F = 0.25, 0.5, 0.75$, and 1. The corresponding pore volumes of the injected gas are also provided. Simulations are for $30 \times 30 \times 30$ lattices.

Figure 48: Total lamellae number density, $\mathcal{N}$, profiles at various snap-off probabilities; (a) $f_{so} = 0$, (b) $f_{so} = 0.5$, (c) $f_{so} = 0.7$, and (d) $f_{so} = 1$. Each figure shows four different stages, where the front approaches the normalized front location at $x_F = 0.25, 0.5, 0.75$, and 1. The corresponding pore volumes of the injected gas are also provided. Simulations are for $30 \times 30 \times 30$ lattices.

Figure 47 shows profiles of snap-off lamellae number density, $\mathcal{N}_{so}$, for the corresponding simulations. In case (a), there is no snap-off lamellae. In cases (b) and (c), snap-off lamellae are generated. The corresponding profiles are similar to the foam saturation profiles of Fig. 46. In case (d), once again the profiles are showing a very stable transition. For this case, about 35% of the throats in the stabilized part of the displaced zone contain snap-off lamellae.

The corresponding plots of total lamellae number density, $\mathcal{N}$, are given in Figure 48. At $f_{so} = 0$ in case (a), it is shown that there are many leave-behind lamellae residing in the system. Profiles are very similar to foam saturation in all cases. One point to notice is that, as the snap-off probability increase, not only more snap-off lamellae are generated (Fig. 47), but also more leave-behind lamellae are created (notice the difference between Fig. 47 and Fig. 48). This is as a result of obtaining a higher fraction of pore bodies swept and consequently having more liquid trapped in the non-invaded throats between the sites.

Figure 49 shows the pressure gradient, $|\nabla P|$, of the system *vs.* pore volume of the gas injected, for the four cases. As expected, case (a) is similar to the drainage process, where gas is displacing liquid. Other cases behave differently. Again, as f_{so} increased, the pressure gradient in the system is increased. The difference is remarkable for case (d), where $f_{so} = 1$. In this case, the pressure gradient in the system is about 20 times higher than for a drainage process (case (a)), and it is about 7 times higher than for a weak foam (case (b)). Also notice that all processes terminate at breakthrough, and the final data show the fraction of the gas injected or the liquid swept. Therefore, as before, the sweep efficiency is much higher for higher f_{so} , and it is very noticeable for a very strong foam (case (d)). In this case, the fraction of swept liquid is about 3.5 times greater than drainage process.

One other aspect to consider in the study of transient foam flow in porous media, is to compare the maximum capillary pressure in the system, ($\Delta P_c = P_g - P_w$), with capillary pressure type of plots of drainage process. This is given in Figure 50 for the four different snap-off probabilities considered before. Given ΔP_c values are in (Pa). These values are estimated assuming an interfacial tension between surfactant solution and gas of $\gamma = 30$ (mN/m), and an average throat radius, $\bar{r}_t = 50$ (μm). Figure 50a is similar to the typical P_c *vs* S_w curves. But as snap-off lamellae are generated, the characteristics of the curves change and the pressure difference increase remarkably. Eventually, it becomes close to a straight line with slope increasing as more liquid is becoming displaced.

Percolation Fraction vs. Percolation Probability Curves

The difference between the presented invasion process and the classical invasion percolation may become more clear by considering the fraction of *accessible* bonds, $P(p)$, plotted *vs.* the throat percolation probability, p_t . In the definition of $P(p)$, accessible is emphasized to state that all the bonds that contain lamellae (and are not open) could be accessible for the flow, therefore, they are part of this fraction. Here, p_t is defined as

$$p_t = \int_{r_{min}}^{\infty} \alpha_t(r) dr \quad (21)$$

Figure 49: Pressure gradient vs. pore volume of gas injected in a $30 \times 30 \times 30$ lattice at breakthrough, for (a) $f_{so} = 0$, (b) $f_{so} = 0.5$, (c) $f_{so} = 0.7$, and (d) $f_{so} = 1$.

Figure 50: $\Delta\mathcal{P}_c$ vs. S_w at four different snap-off probabilities; (a) $f_{so} = 0$, (b) $f_{so} = 0.5$, (c) $f_{so} = 0.7$, and (d) $f_{so} = 1$. Simulations are for $30 \times 30 \times 30$ lattices.

Figure 51: $P(p)$ vs. p_t for different snap-off probabilities; (a) $f_{so} = 0$, (b) $f_{so} = 0.5$, (c) $f_{so} = 0.7$, and (d) $f_{so} = 1$. Simulations are for $30 \times 30 \times 30$ lattices.

where r_{min} is the minimum pore throat size in the invaded phase and $\alpha_t(r)$ is the pore throat size distribution. Figure 51 shows the corresponding plot for previously studied cases. Case (a) is similar to a drainage process with site trapping and no bond trapping in the system. The second condition implies the leave-behind lamellae as mobile lamellae which are accessible for the flow, specially in the next cases. In case (a), the bond percolation threshold is close to the already known value of ~ 0.25 . For the higher values of f_{so} , there is a considerable shift of the percolation threshold to the right of the graph. For instance, if we may use the same terminology, for $f_{so} = 1$, $p_{t,c} \sim 0.92$. According to the above equation, this means that very small pore throats are being invaded (becoming accessible) before breakthrough. This is well expected considering the compact displacement in such cases (see Fig. 40), and it is the main reason for using foam in *EOR*.

3.3.2 Steady-State Displacements

In the study of foam flow in porous media, in addition to finding how the lamellae generation in the system changes the sweep efficiency of the displacement, and what is the minimum pressure gradient for the onset of foam flow, it is also of main concern to find what fraction of the gas will be mobilized when applying a certain amount of pressure gradient. As discussed before, because of snap-off (along with leave-behind) mechanism, the gas phase during the invasion process may be partially (completely) trapped. By applying a sufficient pressure difference in the system, a fraction or all of the trapped gas may be mobilized. This could happen in either the continuous or the discontinuous regimes. Developing our previous model, it is possible to find the fraction of the flowing foam, by applying various pressure gradients. This is the subject of the next study that follows.

Foam Mobilization

At the onset of foam mobilization, the first path to be mobilized was determined and demonstrated in Figs. 40–42. The corresponding minimum pressure gradients to mobilize such paths, in various 2-*D* and 3-*D* lattices, were also given in Fig. 44. The idea behind these findings was to apply an *IPM* type of calculation in the displaced zone, where the *local* capillary forces at the front advance, were also taken into consideration. Then, the minimization of the overall resistance resulted in the identification of the advance location, the minimum overall pressure difference to advance, the determination of the corresponding path, and other information.

In transient displacements, the flowing foam fraction, which is the minimum pressure gradient path's mass fraction, with respect to the overall network size, is not considerable. Basically, even for $f_{so} = 0$, where the path is a fractal object and has a higher mass dimension, it has still a lower dimension than the network's (sites or bonds) mass. As a result, the flowing foam fraction, at conditions when we apply the minimum pressure difference to mobilize the minimum gradient path, goes always to zero, as a larger network is used. This phenomenon also causes the relative permeability of the gas, even in continuous models, to go to zero as a larger lattice is employed. But practically, a higher pressure gradient than the minimum pressure gradient during the displacement may be used. Such a larger pressure gradient, will

mobilize a larger fraction of the foam in the porous media.

It is of interest to investigate this more general issue, which is, what fraction of the gas will be mobilized for a certain amount of pressure difference applied. Again, for simplicity, viscous forces will be neglected, which is a good assumption when we compare with the much higher yield stress type forces involved in this process. The assumptions are as in the transient model. Further, the displacement is continued until all pore bodies in the system are displaced or trapped. Then, the effect of increasing pressure difference at the two opposite ends of such cluster is studied. This is similar to the study of mobilization of *IPM* paths in [77].

By applying a pressure gradient and increasing its value, first the minimum gradient path is mobilized. The value of the minimum pressure gradient and the detailed properties of the path were already discussed. Increasing the pressure gradient above the minimum value, next path that hierarchically needs higher pressure gradient becomes available for mobilization. The effects of previously opened path(s) on this newly available path are neglected. The new path could be a completely independent path, or it can share some portion of the previous path(s), or even it may make a loop with previously opened path(s). Therefore, the size of this path could range from a single pore throat to a very long tortuous path connecting two ends of the network. As the pressure gradient increases, new paths open one at a time until all *accessible* throats in the system are mobilized. The trapped sites in the system and the throats among them are assumed to remain uninvaded. At any step, as a new path becomes mobilized, the fraction of open bonds and sites and the relative pressure gradient data are collected.

In order to identify which path is hierarchically going to be the next path to be mobilized, the novel algorithm presented in [77] is used. The only difference is that, here the clusters by themselves may be different than the those in [77]. The details of the code are not going to be repeated again. Briefly, it is noted that the algorithm uses *IPM* processes to invade the cluster two times, each time starting from opposite sides. Then, an initial guess for the minimum pressure requirement to mobilize all such threshold resistances is made. Later, by finding the minimum throat resistances one-by-one, the process continues. Whenever a complete path (as defined above) forms, the correct and final potential values to the throats are assigned, and the desired data are collected.

As an example, Figure 52 shows a 100×100 lattice at different stages of minimum threshold potential calculation for the entire cluster for a relatively strong foam, where $f_{so} = 0.5$. Three snapshots in the figure are shown: (a) the minimum overall pressure gradients required for mobilization of the sites calculated by *IPM* process starting from the left-hand-side; (b) the same values for *IPM* process starting from the right-hand-side; and (c) the initial guess for overall mobilization potentials found from a combination of the (a) and (b) calculations. In these figures, the dark area shows the trapped liquid sites, grey shows the accessible sites with brightness of grey showing comparatively larger threshold potentials for mobilization.

Having the initial guess of mobilization potentialss of bonds and sites, the mobilized paths are identified one-at-a-time, and the corrections if necessary are made. Figure 53

Figure 52: A 100×100 network, illustrating different steps of finding pressure gradients required to mobilize paths of a previously swept lattice ($f_{so} = 0.5$). The minimum pressure gradient values to reach to the sites by using an *IPM* process started from (a) left-hand-side, (b) right-hand-side. Figure (c) shows the initial prediction of minimum pressure gradients required for mobilization of each site. In all the figures, dark areas are the sites with trapped liquid, and grey areas show the accessible sites. The brighter sites show higher resistance for mobilization.

Figure 53: Pores and bonds in a 100×100 lattice at different stages of mobilization: (a) initial path (minimum resistance path), (b) one third, (c) two thirds and (d) all accessible paths are mobilized. In this simulation, $f_{so} = 0.5$.

shows the mobilized paths at four different stages of mobilization for the same process as in Fig. 52. Here, the pore bodies and bonds of the mobilized part of the lattice are all shown. Fig. 53a shows the first path to be mobilized. Notice that, because of having different process here than in foam invasion, this path could be different than the minimum gradient path at breakthrough. Figures 53(b,c) show the mobilized fraction of sites at different stages, when about one third (b), and two thirds (c) of the bonds are mobilized. Finally Fig. 53d shows the system where all of the accessible bonds and sites of the network are mobilized.

The fraction of mobilized paths in the system by imposing different pressure gradient into the system can now be collected and analyzed. Figure 54 shows the flowing fraction of foam, $\mathcal{X}_f$, vs. the normalized pressure gradient, $|\nabla P|$, for various cases. The parameter in these plots is the snap-off probability. Typically, the mobilized fraction of foam changes similarly for either bonds or sites. Hence, we only show the fraction of the mobilized sites vs. $|\nabla P|$. Snap-off probabilities change to generate very weak to very strong foam. In all cases, whenever a pressure gradient *threshold* is approached, there is a very sharp S-type change in the flowing fraction. This is something expected, but never measured. Below the threshold there is no flowing path. As the threshold is exceeded, suddenly a small increase in $|\nabla P|$ opens many paths in the system. After mobilizing a large fraction of the accessible paths, again the process slows down, and the curves become almost flat. Then, to mobilize more paths, $|\nabla P|$ needs to become much higher.

There is some other information in Fig. 54 that more or less was noticed in previous figures. First, below $f_{so} = 0.35$ (in 2-D), there is no Minimum Pressure Gradient ($|\nabla P|^{min}$) in the system, and mobilization starts from $|\nabla P| = 0$. Second, $|\nabla P|^{min}$ becomes larger as the system's parameter, f_{so} , is higher. Therefore, it is not reasonable to look for one universal $|\nabla P|^{min}$ for all systems, and this value could be as low as zero in weak foams. Finally, after the curves become flat, no further sites can be visited and the remaining sites are the liquid trapped sites. Hence, it can be noticed that as stronger foam is generated, less trapping in the system occurs, and in other words, the sweep efficiency becomes larger.

3.3.3 Application: Sweeping Different Permeability Layers

One of the major reasons of using foam in *EOR* is to block high permeability regions in the reservoirs and divert the injected gas into the lower permeability regions, to increase sweep efficiency. In modeling this behavior, classic invasion percolation once again comes short. But, the presented *IPM* model of foam flow, reasonably simulates cases of displacing different layers with different permeabilities. Here, only two layer systems are tested, by using either weak or strong foam. Obviously, it is simple to extend these simulations to multi-layer systems as well.

For a simple schematic presentation, a two-dimensional lattice is selected. Parallel to flow direction, the lattice is divided into two equal segments of high- and low-permeability regions. The average radius of the throats in the high-permeability region at the top is assigned to be two times greater than the average radius of the throats at the bottom. This makes the permeability of the top region to be about four times greater than the permeability of the

Figure 54: Mobilized Fraction of Foam, $\mathcal{X}_f$, vs. Normalized Pressure Gradient, $|\nabla P|$, in 100×100 lattices. The parameter on the top of the curves shows the snap-off probability values, f_{so} .

bottom region. Now, the displacement takes place from left-to-right.

Figure 55 gives displacement patterns at breakthrough in a 100×100 lattice for a variety of weak and strong foams. For comparison, four different cases for comparison are illustrated. In case (a), where $f_{so} = 0$ and the process is similar to invasion percolation, technically no displacement in the low permeable region at the bottom takes place. The displaced cluster at the top is a self-similar pattern similar to invasion percolation cluster. The minimum gradient path, which in this particular case is the backbone, is presented by a black line inside the light grey invaded cluster. The overall swept fraction of the liquid in this case is less than 0.2. In the next case (b), f_{so} is 0.35 (at the onset of gas discontinuity). In this case, the overall sweep fraction reaches ~ 0.31 . Fig. 55b shows a more displaced cluster, with even some displacement at the bottom. Case (c) shows a well-developed foam. Now, the snap-off probability is 0.5, which is well above the discontinuity threshold for 2-D lattices. The sweep efficiency is very satisfactory, and about 72% of the in-place liquid is displaced at breakthrough. With a very strong foam, an even higher efficiency was obtained. At $f_{so} = 1$, the overall fraction of swept liquid is above 0.84. This case is shown in Fig. 55d.

It is interesting to mention that in case (d), the relative movement of the fronts in two different permeable layers follows a simple relation. The yield stress forces in the two fronts (T_h and T_l) are nearly equal

$$T_h \simeq T_l \quad (22)$$

where subscripts h and l refers to the high- and the low-permeability halves, respectively. Here, we assume that capillary forces are very small and only yield stress forces are dominating in this case, and that the yield stress forces are changing linearly with the front location, X ,

$$X_h \frac{C}{\bar{r}_h} \simeq X_l \frac{C}{\bar{r}_l} \quad (23)$$

Therefore, it is easy to derive

$$\frac{X_h}{X_l} \simeq \frac{\bar{r}_h}{\bar{r}_l} \quad (24)$$

This result can be qualitatively observed in Fig. 55d. Considering the permeability of the layers, K , the above relation can also be written as

$$\frac{X_h}{X_l} \simeq \sqrt{\frac{K_h}{K_l}} \quad (25)$$

It is already known that in percolation, $X_h/X_l \rightarrow \infty$. This is indeed confirmed in Fig. 55a, where $X_l \rightarrow 0$.

One last point to mention is that, the two-layer model presented above considers transient displacement of the foam flow. In case the steady-state mobilization of the foam in two permeable layers is to be studied, the results would be different. Figure 56(a-d) show different snapshots of mobilization for the case when very strong foam with $f_{so} = 1$ is in place. In this figure only mobilized sites of the lattice are shown. It is shown that nearly all the foam in the permeable region becomes mobilized, before any foam in the low permeable region can.

Figure 55: Foam displacement in two-layer porous media, modeled by 100×100 lattices. Snap-off probabilities in the different cases are: (a) $f_{so} = 0$, (b) $f_{so} = 0.35$, (c) $f_{so} = 0.5$, and (d) $f_{so} = 1$. The black lines show the minimum pressure gradient paths at breakthrough. The permeability of the top (half) segment is about four times that of the bottom segment.

Figure 56: Foam mobilization snapshots in two permeable layer porous media, modeled by a 100×100 lattice. The snap-off probability in this case is $f_{so} = 1$. Permeability of the (half) top segment is about four times of the bottom segment.

The reason is that here both layers have the same length. According to equation (23), the yield stress forces in the low-permeable layer of the bottom would be two times higher than in the top layer. Therefore, all the top layer will be mobilized first.

3.4 Conclusions

In this section, a pore network model for transient and steady-state foam flow in porous media was presented for the first time. The model employs the *IPM* process of [77], to consider the yield stress type of resistance of mobilizing lamellae out of the pore throats. Then, along with the local capillary forces of gas invasion at the front, finds the advance site. The model is capable of simulating continuous and discontinuous gas regimes as well. In addition, the mobilization of foam through porous media at steady-state is also investigated. Many interesting results were obtained.

It was shown that, there is not a universal $|\nabla P|^{min}$ for the onset of foam flow in porous media. But depending on the system parameter, here shown by the snap-off probability, $|\nabla P|^{min}$ may vary from zero up to a certain value which itself depends on pore and throat size distributions. Sweep efficiencies of the foam flow for different cases ranging from weak to strong foam were investigated. The liquid sweep fraction is found to be 3.5 times higher for a strong foam compared to a weak (or no) foam. Qualitative presentation of the displacement shows that the foam displacement process is far from being an invasion percolation process. Only for the case $f_{so} = 0$, it is identical to bond-invasion site-occupancy percolation process with bond trapping.

For a continuous gas phase to become discontinuous, a snap-off probability threshold is observed. These values which are different for 2-*D* and 3-*D* lattices, were never reported before. The liquid sweep fraction *vs.* snap-off probability curves were provided for both dimensions. The study also derived the relations between the flowing foam fraction and the pressure gradient imposed on the system. There has been no work reported in the literature in this regard. The effect of different foam qualities on mobilization, by applying progressively different pressure gradients was also obtained.

Finally, this section shows the application of the model in transient displacement of foam in double-permeability layer media. The results are very satisfactory and qualitatively informative. It is shown that in case there is no snap-off lamellae generation in the system, the low permeable region will not be swept. This case is similar to invasion percolation model and the front location ratios agrees with invasion percolation results. For the cases where the gas phase becomes discontinuous, the low-permeable region starts to be displaced. For a very strong foam, a new relation between the front location ratios during displacement is derived.

4 Invasion Percolation with Viscous Forces

B. Xu and Y. C. Yortsos

4.1 Introduction

The displacement (drainage) of a wetting fluid (subscript w) in a porous medium by the injection of another non-wetting fluid (subscript nw), immiscible to the former, has been analysed in great detail in past studies. In the absence of viscous or gravity forces, slow drainage is controlled solely by the capillary pressure, $P_c = P_{nw} - P_w$ (the difference in pressure between the two fluids), which is spatially uniform. At the pore network level, this problem can be modeled by Invasion Percolation (IP), in which the front separating the two fluids advances by penetrating the pore throat at the front with the largest size (smallest capillary resistance). The properties of IP and its close connection to Ordinary Percolation (OP) have been extensively studied [81, 82].

In the presence of gravity [83, 84, 85], or of a gradient in the average pore-size (permeability) [2], slow drainage has been modeled with Invasion Percolation in a Gradient (IPG), which is a modified version of Gradient Percolation (GP) [86]. Here, the capillary pressure varies linearly (or almost linearly) in the direction of displacement, x . Because of their direct relationship (see also below), this gradient also results in a gradient in the percolation probability p , usually expressed in terms of the Bond number, B , ($dp/dx \sim -B$). For example, in invasion in a hydrostatic gradient, $B = \frac{\Delta\rho g_x r_m^2}{\gamma}$, where $\Delta\rho$ is the density difference, g_x is the gravity component in the direction of displacement, r_m is a typical throat size and γ is the interfacial tension between the two fluids. For invasion in a permeability gradient, $B = -\frac{dk^{1/2}}{dx}$, where k is the permeability [2]. In IP ($B = 0$), the entire displacement pattern is a percolation cluster. In IPG, one needs to distinguish two different cases, depending on whether percolation is in a stabilizing or a destabilizing gradient.

In the first case ($B > 0$), for example in the downwards displacement at capillary control of a heavier fluid by the injection of a lighter fluid, or in drainage in a field of decreasing permeability, the percolation probability decreases in the direction of displacement. The region where the invasion has the characteristics of a percolation cluster is only of a finite extent, σ , and was shown in [83], [87] and [84] to scale as

$$\sigma \sim B^{-\frac{\nu}{\nu+1}} \quad (26)$$

where ν is the correlation length exponent of percolation [88, 89]. Here σ denotes the width of the front (in 2-D) or of the front-tail (in 3-D) (see [84] for the necessity for this distinction), where the displacing pattern has the structure of the percolation cluster and fractal concepts apply. Equivalently, σ measures the maximum extent of the correlation length, which in gradient percolation problems becomes finite due to the applied gradient. Various properties of GP and IPG have been studied in considerable detail [83, 90, 91, 92, 2].

In invasion in a destabilizing gradient ($B < 0$), for example in the downwards displacement at capillary control of a lighter fluid by the injection of a heavier fluid, or in drainage in a field of increasing permeability, the percolation probability increases in the direction of displacement. Then, the displacement proceeds in the form of capillary fingers, the scaling of the average thickness of which with (the absolute value of) the Bond number also scales as in (26) [93, 92, 94].

In the presence of both viscous and capillary forces, the displacement is characterized by three dimensionless numbers: the capillary number, $Ca = q\mu_{nw}/\gamma$, where q is the injection velocity and μ_{nw} the viscosity of the displacing phase; the viscosity ratio, $M = \mu_w/\mu_{nw}$, where μ_w is the viscosity of the displaced phase; and the dimensionless system size L (expressed in units of the average pore length l). As Ca or L increase, the viscous pressure drop in the two fluids becomes comparable to capillarity, and one expects that some form of gradient percolation would also describe this process. Work in this direction was reported in the following three studies.

Wilkinson [87] was the first to propose concepts of GP for modeling viscous displacements. He assumed a stabilized displacement and conjectured a power-law scaling between the front extent and the capillary number, of the form $\sigma \sim Ca^{-a}$, where $a = \frac{\nu}{t-\beta+1+\nu}$ and t and β are the OP exponents scaling conductivity and percolation probability, respectively [88]. In a somewhat related study of the drainage of a wetting fluid in an $L \times L$ square lattice, Lenormand [95] delineated the limiting regions in the parameter space (Ca , M and L), where fractal patterns (including percolation) apply. His phase diagram, with the present convention for M , is shown schematically in Fig. 57. He found that a power-law relates the domain boundaries to the system size and obtained the exponents $\frac{\nu}{t+1+\nu}$ or $\frac{\nu}{1+\nu}$, for the percolation-to-compact and the percolation-to-viscous fingering boundaries, respectively. Although not explicitly stated in his paper, Lenormand's work is essentially a study in GP (both in a stabilizing and a destabilizing gradient), as will be shown below. Blunt et al. [96] provided arguments about the extent of the frontal region similar to Wilkinson's, but proposed the different yet exponent $\frac{\nu}{t-\nu+1}$, for the scaling with the capillary number. Interestingly, all these exponents differ from one another, suggesting that a general consensus on this issue has not yet been reached.

The effect of viscous forces on displacements in porous media is of obvious importance to process scale-up and large-scale simulation. As length scales increase, viscous effects are increasingly dominant over capillarity. An understanding of this competition at the pore-network scale is necessary to provide insight on the validity of the conventional continuum description using relative permeabilities, which is standard practice in commercial simulations [97]. Although conventionally used, the very concept of relative permeabilities still remains a subject of debate, particularly in connection to displacements in heterogeneous media [98] and viscous fingering. For example, it is known that under conditions of sufficiently large M and Ca , immiscible displacement becomes unstable (e.g. [99], [100]) and in the large M and Ca limit can be described by DLA (see also Fig. 57). In this paper, we attempt to provide some insight on these problems. We consider drainage in uncorrelated random media in the presence of viscous forces and proceed by postulating an analogy with

Figure 57: Phase diagram for drainage (adopted from [1]).

IPG. Depending on the relative magnitude of M , we anticipate the existence of two different regimes, described by IPG in a *stabilizing* and in a *destabilizing* gradient, respectively. These two regimes control the saturation profiles in the respective displacements. In another sense they also characterize, under dynamic displacement conditions, the percolation-to-compact and percolation-to-DLA transitions described in Lenormand [95] (Fig. 57).

In the stabilized case, the saturation profiles approach a well-known travelling wave state. As in standard GP, we anticipate the existence of a frontal region with the structure of a percolation cluster, but of a finite extent, here limited by viscous gradients, where fractal behavior applies, followed by an upstream region with the characteristics of a compact pattern. To describe the frontal region, we will propose a non-trivial extension of IPG. We show that viscous forces lead to a non-linear relationship between the increment in the percolation probability and the spatial increment, from which the scaling of the front width with the capillary number can be derived. The exponent obtained is identical to Wilkinson's [87], although the two approaches are different. In the destabilized case, we expect that the displacement proceeds in the form of capillary fingers, much like in the displacement of gravity-unstable capillary invasion. Here, we expect that IPG in a destabilizing gradient applies [93]. The exponent scaling the size of the fingers is identical to that obtained by Lenormand [95] for the size dependence of the percolation-to-DLA boundary. Conditions that delineate the validity of these scalings in the two different cases are derived. As the stabilized displacement is also described by the Buckley-Leverett equation (see standard texts, also [87], [101]), the constraint developed applies equally to the Buckley-Leverett formalism. This is the first time that such a condition is reported.

In the stabilized case we also consider the saturation profile near the front. We propose an approximate model based on IPG with a particular percolation probability profile, such that in the front-tail region, ahead of the front, it obeys a power-law with a gradient that *vanishes* at the front, while in the compact region behind the front (at least for 3-D problems), it obeys a different power-law with a gradient that *diverges* at the front. This new version, to be termed Invasion Percolation in a Viscous Gradient (IPVG), is briefly explored. We use numerical simulation to study the corresponding static gradient percolation, to be termed Viscous Gradient Percolation (VGP), based on which we derive scaling estimates for the transversely-averaged saturation. The scaling theory is partially tested with numerical simulation using pore networks and with experiments conducted in model porous media. We conclude with some discussion of the effect of heterogeneity on the continuum description.

4.2 Theory

We consider drainage in a rectilinear porous medium, which is conventionally represented as a random, spatially uncorrelated network of pores (e.g. a rectangular lattice of size $L \times N$ in 2-D or a lattice of size $L \times L \times N$ in 3-D, where N is variable). We take sufficiently large L to suppress finite-size effects at the front, which are particularly important at low rates (see also Xu [102]). We assume a constant lattice spacing l , a variable pore throat size

distribution with probability density function $\alpha(r)$, mean r_m and standard deviation Σr_m , and we take sites of equal volume. The drainage of a fluid of viscosity μ_w by another fluid of viscosity μ_{nw} at the constant volumetric flow rate Q is considered. We take incompressible fluids, thus the total flow rate across any cross-section is constant and equal to the injected, Q . However, this rate is partitioned differently in the two different phases, for example as $Q_w = F_w Q$ and $Q_{nw} = (1 - F_w)Q$, respectively, where the fractional flow term, F_w , is also unknown and must be determined.

In the absence of viscous forces, the capillary pressure is spatially uniform and the displacement proceeds by following the usual rules of IP, namely by successively invading the perimeter pore with the largest size. In the presence of a viscous pressure drop, a gradient in the capillary pressure (negative or positive) is generally expected to develop. In view of the relations

$$P_c = \frac{2\gamma}{r} \quad (27)$$

and

$$p = \int_r^\infty \alpha(r) dr \quad (28)$$

this, in turn, implies a gradient in the percolation probability. Problems involving a constant gradient in p are amenable to GP and IPG, thus we expect that a similar description would also be applicable in the present case involving viscous forces. For example, Fig. 58 shows typical patterns of viscous displacements for $M = 0.1$, obtained from pore network simulation in the absence of trapping (details of the simulation can be found in Haghighi et al. [103] and Xu [102]). When Ca is low (Fig. 58a), viscous forces are negligible and the pattern has the fractal structure of the IP cluster. As viscous forces increase at larger Ca (Fig. 58b), however, the front takes the appearance of a self-affine, rather than a self-similar, curve and it is of a smaller extent. Both trends are consistent with a gradient percolation description.

In general, following GP notions, we distinguish two different cases, one in which the percolation probability (hence P_c) decreases in the direction of displacement, and which has features similar to GP in a stabilizing gradient, and another in which p (hence P_c) increases in the direction of displacement, with features similar to GP in a destabilizing gradient. In our problem, the capillary pressure P_c is controlled by the viscous pressure drop (rather than gravity, as in the case of buoyancy [87]). Therefore, we expect that the viscosity ratio M would play a decisive role in delineating these two regimes. This distinction, also made by Lenormand [95], is fundamental to this paper.

4.2.1 Stabilized Displacement

In the case of a stabilized displacement, we follow [84] and define the mean front position X_c as the place where the transverse average of the percolation probability is equal to the percolation threshold, p_c , namely

Figure 58: Displacement patterns from numerical simulation of drainage in a 100×100 lattice, with $M = 0.1$ and different values of the capillary number: (a) $Ca = 3.2 \times 10^{-4}$, (b) $Ca = 3.2 \times 10^{-5}$, (c) $Ca = 3.2 \times 10^{-6}$ and (d) $Ca = 3.2 \times 10^{-8}$ (IP).

$$p(X_c) = p_c \quad (29)$$

As in the corresponding IPG problem, this front is moving with a velocity v , to be determined. The region near the front is expected to have the properties of GP. More specifically, in 3-D we anticipate the existence of a front-tail region ahead of the front ($X > X_c$), where the invading phase pattern is fractal, followed by a region behind the front ($X < X_c$) (which also includes the “critical region” in the terminology of [87]), where the invading phase occupies a compact region [84] and the conventional continuum description is valid. In 2-D problems, the percolation pattern extends on both sides of the front. A brief sketch of the two regions along with the notation used is shown in Fig. 59. These two regions will be separately analysed. We note in advance that Wilkinson [87]’s analysis is based on the compact regime only, while Lenormand’s [95] is on the fractal regime. For convenience, we will use the term frontal region to denote the region where fractal behavior applies in both 3-D and 2-D geometries, and we will use σ to denote, in units of lattice spacings, its extent, namely the front-tail width or the front width in the respective geometries. In this context, σ also represents the maximum extent of the correlation length, which in gradient percolation is “trapped” to a region of finite extent. Whenever necessary, our emphasis will be on 3-D problems only, to avoid unnecessary complications due to trapping issues associated with 2-D displacements [104].

(i) Frontal Region

The frontal region has width σ and lateral extent L^{d-1} , where d is the embedding dimension. To analyze the displacement in this region, we will focus on two main properties, the scaling of σ and the saturation profile. To proceed, it is necessary that an estimate of the viscous pressure drops in the two phases be derived. Although straightforward when fluids occupy a compact pattern, the problem is more complex when they occupy a fractal pattern, as is the case with the non-wetting phase in this region, where it consists of part of a percolation cluster.

To estimate the pressure drop of the nw phase, ΔP_{nw} , we partition the region in equal size “boxes” of size σ^d and consider the pressure drop across a box. This partitioning is necessary for the application of percolation scalings, and was also used in [84] to estimate the number of sites on the front. Because the displacement pattern is part of a percolation cluster, the dimensionless conductance of the non-wetting phase in the box, G_{nw} , has the percolation scaling [88]

$$G_{nw} \sim \sigma^{-\zeta/\nu} \quad (30)$$

where ζ is the conductance exponent ($\zeta = 1.30$ or 1.12 in 2-D or 3-D, respectively [88, 89]), and it was assumed that the system size is sufficiently large in any one dimension for these scalings to be applicable. The exponent ζ is simply related to the conductivity exponent t used in the previous studies, $t = \zeta + (d - 2)\nu$, thus the two coincide in 2-D geometries. The

Figure 59: 2-D Schematic of the 3-D front region and the notation used.

nw phase volume flow rate across each box, $Q_{i,nw}$, is determined from the overall volume flow rate, Q_{nw} , by a simple mass balance

$$Q_{i,nw} = \frac{Q_{nw}\sigma^{d-1}}{L^{d-1}} \quad (31)$$

Combining (30) and (31) gives the following estimate for the pressure drop of the nw phase across the frontal region

$$\Delta P_{nw} = \frac{AQ_{nw}\mu_{nw}}{L^{d-1}r_m^3}\sigma^{\frac{\zeta}{\nu}+d-1} \quad (32)$$

where A is a dimensionless constant of order 200 [105, 83], and we implicitly used a Poiseuille law model for the conductance across a pore.

For further progress, an expression for Q_{nw} is required. To proceed we will postulate that quantities at the front reach a steady-state in a coordinate system moving with the front velocity, v . The approach of stabilized immiscible displacements to a travelling-wave state is a well-known fact and has been established theoretically (for example, see [87, 106]) and experimentally. A subsequent mass balance on the nw phase in the frontal region leads after some calculations to the result

$$Q_{nw} = \phi v L^{d-1} l^2 S_{nw} \quad (33)$$

where ϕ is porosity, and the saturation, S_{nw} , is the transverse average of the fraction of sites occupied by the nw phase. Now, in the region under consideration, the displacing phase consists of a part of the percolation cluster, thus we further expect the scaling $S_{nw} \sim \sigma^{D-d}$, where D is the mass fractal dimension. Then, Equation (33) becomes

$$Q_{nw} = B v L^{d-1} l^2 \sigma^{D-d} \quad (34)$$

with B a dimensionless constant. At this point, we must emphasize the difference between this approach and Lenormand's [95], where the entire injected rate Q is used in the calculation of the pressure drop. By contrast, (34) implies that only a small fraction of Q actually reaches the frontal region, at least under conditions of a travelling state of constant velocity. This difference will be ultimately reflected in the scaling exponents to be derived.

Determining the magnitude of the velocity requires the solution of the overall problem, including the consideration of the region away from the front. The specific approach involves the solution of the Buckley-Leverett problem and it is discussed in various standard references (see also [87, 101]). For the purposes of this section, however, it suffices to note the simple scaling result, $v \sim Q/L^{d-1}l^2$, to leading-order independent of the capillary number. Thus, using (34) we may express (32) as

$$\Delta P_{nw} = \frac{C v l^2 \mu_{nw}}{r_m^3} \sigma^{\frac{\zeta+\nu(D-1)}{\nu}} \quad (35)$$

where $C = AB$. Equation (35) shows that because of the fractal nature of the displacing phase, the viscous pressure drop in the nw phase scales *non-linearly* with the width of the

front. This dependence leads ultimately to a non-trivial difference with the GP, as will be shown below.

The estimation of the pressure drop of the wetting phase is straightforward. We note that the displaced phase is compact (certainly in 3-D and also in 2-D pore networks of sufficiently high lattice coordination number for the two phases to co-exist), hence we can use continuum theory. Making use of Equation (31), with an obvious change in notation, of the corresponding continuum scaling, $G_w \sim \sigma^{D-2}$, and taking to leading-order in this region the approximation $Q_w \approx Q$, gives the following estimate

$$\Delta P_w = \frac{Dql\mu_w}{r_m^2}\sigma \quad (36)$$

where the constant D is of the same order as C , and we also introduced the mean flow velocity, $q = Q/L^{d-1}l^2$. Finally, combining (35) and (36) gives the variation of P_c across the front

$$\Delta P_c = \Delta P_{nw} - \Delta P_w = \frac{Cvl^2\mu_{nw}}{r_m^3}\sigma \left(\sigma^{\frac{\zeta+\nu(D-2)}{\nu}} - bM \right) \quad (37)$$

where we introduced the $O(1)$ constant $b \equiv \frac{qr_mD}{vlC}$. It is important to note that the ratio q/v is $O(1)$, but it also decreases with M , as dictated by the Buckley-Leverett solution. For the stabilized displacements assumed in this section, the RHS of (37) must be positive, namely we must have $\sigma^{\frac{\zeta+\nu(D-2)}{\nu}} - bM > 0$. For a fixed M , this is possible at sufficiently large σ . More precise criteria are discussed in a later section.

We consider, next, the variation in p . By using Equations (27) and (28) we obtain

$$\Delta P_c \approx -\frac{2\gamma\Delta r}{r_m^2} \approx \frac{2\gamma\Sigma\Delta p}{r_m^2} \quad (38)$$

where all increments are in the direction of displacement, and combining with (37) we find

$$\Delta p \approx \frac{Ca_F Cl^2}{2\Sigma r_m^2}\sigma \left(\sigma^{\frac{\zeta+\nu(D-2)}{\nu}} - bM \right) \quad (39)$$

where the modified capillary number, $Ca_F \equiv \frac{\nu\mu_{nw}}{\gamma}$, is based on the front velocity (see also [87]). Equation (39) shows that in contrast to standard GP and IPG (for example, when gradients are provided by buoyancy), the change in the percolation probability in the viscous problem is *not* linearly related to the size of the increment. Nonetheless, we can still obtain the scaling of the front width by applying the self-consistency argument of gradient percolation [87, 84]. Indeed, as σ delineates the extent over which percolation scalings apply, we also have

$$\Delta p \sim \sigma^{-\frac{1}{\nu}} \quad (40)$$

Combined with (39), this yields the algebraic equation

$$\sigma^{\frac{1}{\nu}+1} \left(\sigma^{\frac{\zeta+\nu(D-2)}{\nu}} - bM \right) \approx \frac{2\Sigma}{Ca_F C} \quad (41)$$

where we absorbed into C a constant of $O(1)$. The solution of this equation gives the scaling of the front width as a function of Ca and M . For typical values in 3-D, this equation reads

$$\sigma^{2.14} (\sigma^{1.77} - bM) \approx \frac{2\Sigma}{Ca_F C} \quad (42)$$

Numerical results will be presented below. It is immediately obvious that the scaling to be obtained is different from the standard GP problem, which in this case arises only if the term in parentheses in the LHS of (41) and (42) is equal to one.

Perhaps of more interest is the asymptotic behavior of the solution at large σ (recall also the assumption of large σ implicit to the derivation of (41)), which is expected to be the case at relatively small Ca_F . This case is formally obtained if we assume that most of the pressure drop occurs in the displacing nw phase and we neglect the pressure drop in the displaced phase. For example, this assumption was made by Lenormand [95] in delineating the percolation-to-compact boundary, and it is also implicit in the analysis of Wilkinson's [87]. Then, Equation (39) reads

$$\Delta p \approx \frac{Ca_F C}{2\Sigma} \sigma^{\frac{\zeta+\nu(D-1)}{\nu}} \quad (43)$$

which in conjunction with (40) leads to the asymptotic result

$$\sigma \sim \left(\frac{Ca_F C}{2\Sigma} \right)^{-\frac{\nu}{1+\zeta+\nu(D-1)}} \quad (44)$$

Equation (44) expresses the asymptotic scaling of the front (or front-tail) width with Ca_F for the case of a stabilized displacement. Fig. 60 shows the numerical solution of (41) for typical parameter values in 3-D geometries. The asymptotic approach of the full solution to this scaling at small Ca is apparent. We note that the region of validity of (44) extends over several decades in Ca_F and will be taken as the predominant scaling result. Fig. 60 also shows that at relatively large Ca the front width approaches a constant. However, the validity of the percolation expressions in this limit is questionable, and this behavior will not be considered.

As in the previous studies (Wilkinson [87], Lenormand [95] and Blunt et al. [96]), the scaling (44) is a power law. In fact, the exponent $\frac{\nu}{1+\zeta+\nu(D-1)}$ is *identical* to Wilkinson's, $\frac{\nu}{1+t-\beta+\nu}$, if we substitute ζ in terms of t and make use of the well-known percolation relation, $D = d - \beta/\nu$. This exponent would also have coincided with Lenormand's for the scaling of the percolation-to-compact boundary, had we assumed $Q_{nw} = Q$ at the front, which in the present context is tantamount to taking $D = 2$. As shown below Wilkinson's result was obtained differently, by extrapolating in the frontal region the *continuum* solution valid behind the front. The fact that the present work reproduces his result shows that the two approaches are consistent in this case of stabilized displacements.

Figure 60: Numerical solution of (41) vs. modified capillary number for three different values of M .

Using accepted estimates, the exponent in (44) is equal to 0.382 or 0.25 in 2-D or 3-D, respectively. The rather small values suggest a weak sensitivity of σ on Ca_F , C and Σ . It should be kept in mind that the rate dependence in Ca_F has entered through the front velocity, v . This can be of some significance in investigating the effect of M , which also influences v (see also below and [101]). It is also interesting to note that as the degree of heterogeneity, Σ , increases the front width increases. In fact, Equation (44) suggests that for these displacements it is more appropriate to use a modified capillary number involving the product $\gamma\Sigma$. Finally, we must also note that the scaling (44) can also be obtained by using an extended version of GP, termed Viscous Gradient Percolation (VGP), to be introduced below for modeling the saturation profile. However, although necessary for the saturation profile, VGP is not required for the derivation or the validity of the power-law (44).

(ii) Compact Region

Behind the front, the previous theory is no longer applicable, as the displacement patterns are Euclidean and fractal notions do not apply. Locally, however, the displacement is still controlled by capillarity, assuming sufficiently low Ca . We proceed by assuming that the injection rates are sufficiently small, for gradients in volume-averaged quantities to be small, so that volume averages are meaningful. Conditions for the validity of this assumption are developed in a later section. Then, we may proceed with the standard continuum description [106, 87], in which the individual phase velocities obey an extended Darcy's law

$$\mathbf{q}_i = -\frac{k k_{ri}}{\mu_i} \nabla P_i \quad \text{for } i = w, nw \quad (45)$$

and capillary equilibrium applies

$$P_{nw} - P_w = P_c(S_{nw}) \quad (46)$$

Here, the relative permeabilities, k_{ri} , and the capillary pressure, P_c , are functions of the saturation, S_{nw} , in principle computable from the simulation of an IP process for $p > p_c$. Heiba et al. [107] and Sahimi and Siddiqui [108] have calculated such functions for Bethe and regular lattices, respectively, using OP, while Wilkinson [87] has described their asymptotic behavior. According to this approach, the relative permeability functions of the two phases are computed as the relative conductances of the two phases ("occupied" and "empty"), randomly distributed following the occupancy patterns of OP (although a more appropriate description should be based on occupancy patterns involving IP with trapping [81]). In either case, the scales are separated and a standard continuum argument can be used to lead to the following well-known equation for the description of 1-D displacements

$$\phi \frac{\partial S_{nw}}{\partial t} + q \frac{\partial f_{nw}(S_{nw})}{\partial x} = \frac{\partial}{\partial x} \left(\frac{k k_{rw} f_{nw}}{\mu_w} \frac{\partial P_c}{\partial x} \right) \quad (47)$$

where the fractional flow

$$f_{nw} = \left(1 + \frac{k_{rw}\mu_{nw}}{k_{rnw}\mu_w}\right)^{-1} \quad (48)$$

and the capillary pressure $P_c = \frac{\gamma J(S_{nw})}{\sqrt{k}}$ are functions of S_{nw} . For homogeneous systems, we can further write

$$\phi \frac{\partial S_{nw}}{\partial t} + q \frac{\partial f_{nw}(S_{nw})}{\partial x} = \frac{\partial}{\partial x} \left(D(S_{nw}) \frac{\partial S_{nw}}{\partial x} \right) \quad (49)$$

where the diffusion coefficient is $D = \frac{\gamma \sqrt{k} k_{rw} f_{nw}}{\mu_w} \frac{dJ}{dS_{nw}}$. A direct consequence of the continuum description is that the relevant length scale for saturation changes, hence of the upstream region of the front, is $\sqrt{k}Ca^{-1}$. The difference in the scaling exponents in the two regions suggests much sharper saturation profiles in the compact regime compared to the frontal region. At the same time, saturation gradients must be sufficiently small for volume-averaged quantities, such as saturation and relative permeability, to be defined. The validity of this is discussed in a later section.

In a subset of the compact region adjacent to the front (the “critical region” of [87]), percolation theory can be applied to provide the asymptotic behavior of the relative permeability and capillary pressure functions in terms of S_{nw} at small S_{nw} . Based on this behavior and assuming a travelling-wave solution, Wilkinson solved the continuum equation (49) to obtain the local profile of saturation in that region. In our notation, his result reads

$$S_{nw} \sim \left(\frac{Ca_F C}{\Sigma} (X_0 - X) \right)^{\frac{\beta}{1+\beta}} \quad (50)$$

where we also included the heterogeneity factor Σ , and the previous comment on the effect of v still applies. From (50) it is straightforward to obtain the profile of the percolation probability in this region

$$\Delta p \sim \left(\frac{Ca_F C}{\Sigma} (X_0 - X) \right)^{\frac{1}{1+\beta}} \quad (51)$$

where the percolation result $S_{nw} \sim \Delta p^\beta$ was also used. In [87], X_0 was defined as the “leading edge of the front”.

Before we proceed, we must point out that if we adopt the definition of [87] for X_0 , from which it also follows that $X_0 > X_c$ (in fact, $X_0 \approx X_c + \sigma$), Equations (50) and (51) cannot be strictly valid, as the region of integration includes the front-tail region ($X_c < X < X_0$), where the continuum equations do not apply. In fact, it would probably be more accurate to modify these equations by defining $X_0 \equiv X_c$ (indeed, in our definition, X_c is the place where $p = p_c$) and to accept their validity only in the critical region $X < X_c$. This will be considered below in modeling the saturation profile. In their present form, Equations (50) and (51) must be viewed as an approximate composite solution that spans both the fractal and the compact regions, although it does approach asymptotically, in the far-field, the correct continuum scaling (50).

Equation (51) was used in [87] to obtain an estimate of the front-tail width, by proceeding in essentially the following fashion: Evaluating (51) at $X = X_c$ and taking $\sigma = X_0 - X_c$ gives

$$\Delta p \approx \left(\frac{Ca_F C \sigma}{\Sigma} \right)^{\frac{1}{1+t-\beta}} \quad (52)$$

which is the counterpart of our equation (43). Although both power-laws, the two equations have different exponents. In fact, the exponent of (43) is always greater than one, whereas that of (52) is always smaller than one. Moreover, the dependence of Δp (hence of ΔP_c) on Ca is different (linear vs. non-linear). To obtain the scaling of σ with Ca the previous argument is applied, using (40) in (52). After some calculations, we obtain

$$\sigma \approx \left(\frac{Ca_F C}{\Sigma} \right)^{-\frac{\nu}{1+t-\beta+\nu}} \quad (53)$$

which, in view of the relation between t and ζ , is *identical* to our Equation (44). The coincidence of the two exponents is rather remarkable, given that one approach uses scaling laws in a fractal region, while the other is based on a continuum description, and that, as mentioned above, the various profiles are markedly different in the two cases. The fundamental reason for the coincidence of the two results is that the front width σ also happens to be the length of the interval ξ where the overall capillary pressure difference, ΔP_c , is the same in both approaches. Indeed, if we equate the associated two expressions for ΔP_c (or, equivalently, Δp) over an increment ξ , we have

$$Ca_F \xi^{\frac{t-\beta+\nu}{\nu}} \sim (Ca_F \xi)^{\frac{1}{t-\beta+1}} \quad (54)$$

This equation has the solution $\xi \sim Ca_F^{-\omega}$, where ω is the previous exponent, $\omega = \frac{\nu}{1+t-\beta+\nu}$, hence also $\xi \sim \sigma$.

(iii) Saturation Profile

Equation (44) (or (53)) provides the scaling of the front width with Ca . The other important quantity in gradient percolation is the saturation profile. Gouyet et al. [84] and Hulin et al. [91] discussed scaling properties of saturation profiles for the classical GP and IPG problems. As already mentioned, in these problems the percolation probability increment across a region scales linearly with its extent. As it is clear from equations (43) and (51), however, this is not the case for the present problem. We recall that in Equation (43), Δp expresses the variation of p across the frontal region, where patterns are fractal, where in Equation (51) (and under the definition $X_0 = X_c$) it expresses the variation across the increment $X_c - X$, where patterns are compact. To proceed, we first note that it is not difficult to generalize (41) to arbitrary (but suitably constrained) increments, $\xi \equiv X - X_c > 0$ with $\xi < \sigma$, and write

$$\Delta p \approx \frac{Ca_F C}{2\Sigma} \xi \left(\xi^{\frac{\zeta + \nu(D-2)}{\nu}} - bM \right) \quad (55)$$

for the variation of p across such an increment. This could be further approximated by

$$\Delta p \approx \frac{Ca_F C}{2\Sigma} \xi^{\frac{\zeta + \nu(D-1)}{\nu}} \quad (56)$$

Using (51) and (56) we may now analyze the saturation profile near the front, on either side of X_c . For the remainder of this section, our analysis will be restricted to 3-D geometries.

To approximately describe the saturation profile, we will propose a model GP in which the percolation probability has the profile suggested by equations (51) and (56). A schematic of the resulting composite profile of p is shown in Fig. 61. This profile has the form of a “double hump”, with the probability gradient at p_c *vanishing* as we approach X_c from the right, but *diverging* as we approach it from the left. This feature is different from IPG, where the gradient at p_c is constant. In reality, of course, the actual dependence of the profile near p_c is not as extreme as indicated by the above limits. In fact, corrections, on either side of X_c are probably necessary. For example, one could use the more appropriate equation (55) to describe the approach to p_c from the right. However, we expect that these will exert only second-order effects on the saturation profile and for this reason will not be considered (although they are important for delineating the validity of this regime, as will be discussed below). The particular profile depicted in Fig. 61 gives rise to a rather novel GP problem, to be termed Viscous Gradient Percolation (VGP). To understand its features, a brief study was conducted.

Viscous Gradient Percolation (VGP)

We consider a static percolation problem in a lattice with a percolation probability gradient that vanishes at the percolation threshold from the right and diverges from the left, namely

$$p - p_c = \begin{cases} -B(X - X_c)^a & \text{for } X > X_c \\ (B(X_c - X))^c & \text{for } X_c \geq X \end{cases} \quad (57)$$

Here, $B > 0$ denotes an equivalent Bond number, exponents $a > 1$ and $0 < c < 1$ are arbitrary, and capital letters denote distances in lattice units. However, in the specific problem under consideration, we have $a = \frac{\zeta + \nu(D-1)}{\nu}$, and the two exponents are related through $c = \frac{1}{1 + \nu(a-1)}$. We conducted numerical simulations for this gradient percolation problem for various values of a , and specifically for $a = 2.80$, which corresponds to 3-D. Fig. 61 shows probability and saturation (transversely-averaged occupancy) profiles plotted vs. normalized distance for two different values of B . The overall features of the saturation profiles are similar to GP: the profile decreases almost linearly with distance in the region upstream of the front, and the front extent increases as B decreases. (The different lattice sizes used in the normalized plots of these figures should be noted). However, in the VGP problem we notice some additional features: the region near the front is of a larger extent, the saturation

Figure 61: Percolation probability (dashed line) and saturation (solid line) profiles vs. normalized length, for 3-D VGP: (a) $B = 2 \times 10^{-4}$ in a lattice of $300 \times 300 \times 2X_c$, (b) $B = 10^{-6}$ in a lattice of $300 \times 300 \times 2X_c$.

Figure 62: Scaling of the front width with Bond number in 3-D with $a = 2.80$ involving 50 seeds. The best-fit line gives a slope of -0.234. The theoretical value is -0.254.

varies more slowly with distance downstream of the front (the front-tail region) and has a “bent knee-like” shape. Some of these features also appear in the low rate experiments to be discussed below. For quantitative comparisons, we computed the front width σ using the definition of Gouyet et al. [84]. Fig. 62 shows a log-log plot of σ vs. B for 3-D VGP. The results indicate a power-law relationship with a slope of -0.232. Similar power-law relationships were also found for other values of a tried in a related problem (Xu [102]).

To interpret the above findings we applied an extension of the theory of GP to the present case. By applying the self-consistency argument of GP, a power-law scaling for the front width with B can be obtained. Indeed, using the percolation scaling $p_c - p \sim \sigma^{-1/\nu}$ and substituting $X - X_c \sim \sigma$ in the top member of Equation (57) (recall that in 3-D the fractal region lies only to the right of X_c), readily leads to the following power-law scaling

$$\sigma \sim B^{-\frac{\nu}{1+a\nu}} \quad (58)$$

It is worth noting, however, that an *identical* power law would have also been obtained, had we used the lower member of Equation (57), namely had we extended the definition of σ upstream of X_c and made use of the scaling (40) in the compact regime upstream of X_c . Essentially, this was the approach taken by Wilkinson [87]. Again, this remarkable coincidence is due to the specific relation between a and c and has the same interpretation given above. This also implies that the scaling law (58) remains valid even for the 2-D case, where fractal behavior is displayed on both sides of the front.

Equation (58) confirms the numerical dependence found in Fig. 62, and generalizes the GP result (26) to arbitrary exponents. Similar results were also obtained for a simpler profile we used in a previous version of this paper, in which the behavior of p across X_c was anti-symmetric [102]. Comparison of the theoretical slope of -0.254 with the simulations of Fig. 62 shows good agreement between theory and simulation. We conclude that the scaling in (58) is a valid generalization to VGP of the GP results of Gouyet et al. [84]. We also note that as a increases, the sensitivity of σ to B weakens, while its magnitude increases. This is of importance to the 3-D viscous problem where a is relatively large, $a = 2.80$.

Proceeding as in Gouyet et al. [84] it is also straightforward to derive the following scaling for the saturation

$$S_{nw} \sim p B^{\frac{\beta}{1+a\nu}} \Pi_f^{(a,c)} \left(\frac{X_c - X}{\sigma} \right) \quad (59)$$

where $\Pi_f^{(a,c)}(u)$ is a generalization of the scaling function of GP and depends on a and c , in general. Properties of the function $\Pi_f^{(1,1)}(u)$ were discussed in Gouyet et al. [84], who identified a different asymptotic behavior depending on the value of u :

When $u > 0$, the function approaches the ordinary percolation scaling, $\Pi_f^{(1,1)}(u) \sim u^\beta$. When $u < 0$, the function is approximately described by the best-fit expression

$$\log \Pi_f^{(1,1)}(u) = -1.1u^2 + 0.48u + 0.10 \quad (60)$$

To test the theoretical prediction (59) we used numerical simulation. Fig. 63 shows plots of $S_{nw}/p B^{\frac{\beta}{1+a\nu}}$ vs. the rescaled distance u for $u < 0$, for various values of the Bond number B . For a fixed exponent a , but for variable B , all data are shown to collapse to a single curve. This collapse confirms the scaling in (59) in the interval $u < 0$. The simulations of Fig. 63 can be fit with the best-fit expressions

$$\log \Pi_f^{(2.80,0.38)}(u) = -4.04u^2 - 0.64u + 0.17 \quad (61)$$

The difference with the GP expression (60) reflects the extended tail of the saturation profile near the front in VGP. For $u > 0$, $\Pi_f^{(a,c)}(u)$ was found to approach for any a the ordinary percolation expression, $\Pi_f^{(a,c)}(u) \sim u^{c\beta}$, which is the correct asymptote in the critical region, thus also confirming the validity of (59) in that interval. Expressions for the function Π_f for

Figure 63: Normalized saturation profiles vs rescaled distance in 3-D VGP for four different Bond numbers in the range 2×10^{-4} to 2×10^{-6} and for lattice sizes $300 \times 300 \times 2X_c$.

a percolation probability profile which is antisymmetric around X_c can be found in [102]. We conclude that VGP leads to an extended tail near the front, but otherwise obeys scaling laws that can be obtained by a direct generalization of the classical GP approach.

Consider, now, the application of the above to the viscous displacement problem. We proceed with the assumption that IPVG follows the same scaling as in the static VGP process, which is the same assumption used in connecting IGP and GP [91]. This assumption requires the absence of trapping, hence it should be applicable in the frontal region (at least for the 3-D problem) of interest to this section. Then, by making in (58) the substitution $B \sim Ca_F C / \Sigma$ we obtain

$$\sigma \sim \left(\frac{Ca_F C}{\Sigma} \right)^{-\frac{\nu}{1+\zeta+\nu(D-1)}} \quad (62)$$

which is identical to the scaling obtained previously. It is interesting to note that this scaling can also be obtained by using the standard GP argument, but with a different Bond number, $B = |\nabla p| \approx Ca_F^{\frac{1+\nu}{1+\zeta+\nu(D-1)}}$.

We summarize this section by emphasizing the different description of percolation processes involving viscous forces in the two regions, near and away from the front, at least for relatively low Ca . The different scalings, $Ca_F^{-\frac{\nu}{1+\zeta+\nu(D-1)}}$ and Ca^{-1} , obtained indicate that near the front, the continuum description (49) for the profile should be replaced with the more appropriate VGP Equation (59). Either theory suggests an advancing front. In the VGP model, the profile is a function of $X - X_c$, Ca and M , the time-dependence entering through X_c , which varies linearly in time. A travelling state with constant velocity is also contained in the continuum description (49). However, the latter predicts a *hypodiffusive* behavior (de Gennes [106]), namely a profile with a divergent derivative at the front (a sharp “knee”), in contrast to the more “bent knee-like” predictions of VGP. Thus, appropriate caution must be exercised in using the continuum approach in this region.

(iv) Region of Validity of Stabilized Displacements

The above scaling was obtained under the assumption that the displacement is stabilized. At a minimum, this implies that the RHS of (37) and (39) must be positive. Thus, to within a constant, a necessary condition is

$$bM < \left(\frac{Ca_F C}{2\Sigma} \right)^{-\frac{\zeta+\nu(D-2)}{1+\zeta+\nu(D-1)}} \quad (63)$$

However, this is not sufficient. For the stabilized displacement assumed here, the percolation probability must be decreasing in the direction of displacement over all increments $\xi < \sigma$. Comparison with the generalized expression (55), shows that the following constraint

$$bM < \xi^{\frac{\zeta+\nu(D-2)}{\nu}} \quad \text{for } \xi < \sigma \quad (64)$$

must be satisfied. Clearly, this requires that M be sufficiently small. This condition is implied in Lenormand's [95] description of the validity of the percolation regime which indicates a transition at $M = 1$. Of course, condition (64), based on statistical physics scalings, is only valid above a certain cutoff, ξ_c , in which case it reads

$$\frac{q}{\phi v} M < \xi_c^{\frac{\xi + \nu(D-2)}{\nu}} \quad (65)$$

where we made use of the definition of b and set to 1 the $O(1)$ constant. For example, for the arbitrary value $\xi_c = 5$, the above reads

$$\frac{qM}{\phi v} < 5^{1.77} \approx 17 \quad (66)$$

where we made use of the definition of the various constants. In view of the fact that in Buckley-Leverett displacements, the ratio $\frac{\phi v}{q}$ is greater than one and in fact increases with M , the above constraint is satisfied for values of M larger than would have been expected.

Nonetheless, a transition will occur at a finite M . This can be inferred by considering the limit of the front velocity at large M . The Buckley-Leverett condition for the front velocity is

$$\frac{\phi v}{q} \equiv \frac{df_{nw}}{dS_{nw}} = \frac{f_{nw}}{S_{nw}} \quad (67)$$

where the fractional flow function is

$$f_w = \frac{1}{1 + \frac{\kappa(S_{nw})}{M}} \quad (68)$$

and κ is the ratio of the wetting to non-wetting relative permeabilities. Now, at large M , we expect that the saturation upstream of the front, $S_{nw,F}$ is small. In fact, in view of the behavior $\kappa \sim S^{-\frac{\beta}{\beta-1}}$, the solution of (67) is

$$S_{nw,F} \sim M^{-\frac{\beta}{\beta-1}} \quad (69)$$

This means that at large M the ratio κ/M is finite, therefore, (65) leads to a condition of the form

$$M^{1-\frac{\beta}{\beta-1}} < const \quad (70)$$

Fig. 64 shows a plot of the LHS of (66) vs. M for typical values in 3-D, where the existence of a finite M for a given cutoff is indicated. The existence of a relatively sharp constraint on M for the validity of the stabilized displacement, namely of the often used Buckley-Leverett equation, is an important result of this section.

Figure 64: Plot of the LHS of (66) vs. M .

4.2.2 Capillary Fingering

When condition (65) is violated, for example when the nw fluid has a much smaller viscosity, most of the pressure drop occurs within the displaced phase. Equation (55) shows that in such cases p increases in the direction of displacement. IPG problems with spatially increasing probability profiles involve a negative Bond number, and were classified as invasion in a destabilizing gradient [93, 92]. In particular, capillary invasion in a destabilizing gravity field, for example corresponding to the release of a lighter fluid at the bottom of a porous column filled with a heavier fluid, was studied in considerable detail [93] (see also the related problems of [94] and [2]). In these studies it was found that the displacement occurs in the form of distinct capillary (but not DLA-type) fingers. For a sufficiently long column, one single finger emerged. Fig. 65 reprinted from Chaouche et al. [2], shows the structure of such a finger for capillary invasion in a field of increasing permeability. Scaling arguments similar to the self-consistency arguments of GP can also be used here [87, 93] to show that this finger is essentially a string of beads of average width σ with the following scaling behavior

$$\sigma \sim |B|^{-\frac{\nu}{\nu+1}} \quad (71)$$

To apply these findings to the viscous problems of interest here, an expression for B is needed.

To proceed, we first estimate ΔP_c (and Δp) across an element of size σ^d in the geometry of Fig. 65. Note that, in contrast to the stabilized displacement, where it spans the entire cross-section of the sample of area $\sim L^{d-1}$, here the nw phase occupies narrow fingers. Thus, the appropriate expression corresponding to (32) is

$$\Delta P_{nw} = \frac{AQ_{nw}\mu_{nw}}{r_m^3} \sigma^{\frac{\xi}{\nu}} \quad (72)$$

where $Q_{nw} = Q = qL^{d-1}l^2$. However, the equation for the pressure drop of the w phase remains as in (36). After some manipulations we obtain the following equation for the variation of p across an increment of size σ ,

$$\Delta p \approx \frac{ACal^2}{2\Sigma r_m^2} \sigma \left(L^{d-1} \sigma^{\frac{\xi-\nu}{\nu}} - b'M \right) \quad (73)$$

where $b' = \frac{Dr_m}{Al}$ is an $O(1)$ constant. We may now identify the Bond number for this problem, by assuming that the last term within the parentheses of the RHS of (73) is the dominant term, namely

$$B = -\frac{DCaMl}{2\Sigma r_m} \approx -\frac{DCaM}{2\Sigma} \quad (74)$$

This assumption is equivalent to neglecting the pressure drop in the displacing phase (as also done by Lenormand [95]). Then, directly comparing with (71) gives the final result

Figure 65: Single finger in GP in a destabilizing gradient (from [2]).

$$\sigma \sim \left(\frac{DCaM}{2\Sigma} \right)^{-\frac{\nu}{\nu+1}} \quad (75)$$

This power law has the familiar GP exponent, which takes the values 0.571 or 0.469 in the respective geometries (compared to 0.382 or 0.25 of the previous case). The exponent is identical to Lenormand's [95] for the scaling of the percolation-to-viscous fingering boundary (see Fig. 57), although his exponent did not pertain to the width of a finger, or to the particular regime of destabilizing GP discussed here. (However, it was pointed out that the transition would eventually result in fingers continuously thinning as the DLA regime is approached). Comparison with (44) shows that the scaling exponent almost doubles as the mobility ratio increases from the one limiting regime to the other, thus implying a higher sensitivity on the capillary number.

Equation (75) shows that the finger width decreases with an increase in the capillary number Ca and the mobility ratio M , and that it eventually reduces to a single thin finger of the size of a single pore (and where the above scaling fails and a DLA regime emerges). This conclusion was also reached qualitatively by Lenormand, although he did not provide the specific dependence of the finger width on the relevant parameters. We also need to point out that because of its particular exponent, equation (75) can be approximated rather well (at least in 3-D) with the expression

$$\sigma \sim Ca^{-0.5} \quad (76)$$

This scaling is consistent with that of the fastest (most dangerous) growing finger predicted by the linear stability analysis of Chuoke et al. [99, 109], which suggests a $1/2$ exponent, although the two should not be confused. The present analysis is based on finger widths of the order of the pore-scale, while the linear stability analysis of [99] is actually based on a continuum description of stabilized displacements, using an ad hoc expression for the interfacial behavior in the form of an effective macroscopic interface.

A necessary condition for the validity of scaling (75) can be readily derived by requesting $\Delta p < 0$ in (73), namely $L^{d-1} \sigma^{\frac{\zeta-\nu}{\nu}} - b'M < 0$. This leads to the following condition

$$Ca^{-\frac{\zeta-\nu}{1+\zeta}} L^{\frac{(d-1)(\nu+1)}{1+\zeta}} < M \quad (77)$$

within constants of $O(1)$. Based on (77) we can make the following remarks:

1. As Ca increases, the regime of capillary fingering is reached at smaller values of M , (although one should note that the exponent of Ca is rather small, and equals 0.11).
2. Condition (77) is different from (70) which delineates the limit of validity of a stabilized displacement. Obviously, between these two regimes there must exist an intermediate regime with more complex scaling. Additional work to explore the characteristics of this regime is needed.
3. The lattice size L (or, in the case of multiple fingers, the spacing between the fingers, W) enters explicitly in the above condition. In the case of several fingers of spacing W , this

condition remains the same, with W in place of L . In the latter case, one could advance the argument that (77) actually defines the finger spacing, namely that

$$W = Ca^{\zeta-\nu} M^{\frac{1+\zeta}{(d-1)(\nu+1)}} \quad (78)$$

Such a conjecture would imply that the percolation probability always remains near p_c , an idea consistent with self-organized criticality arguments. However, additional work is needed in this direction. Likewise, more work needs to be done to explore the saturation profile in this case.

The above analyses show that the displacement behavior is different depending on the relative magnitude of M . This is a direct consequence of the different expressions used for the pressure drop in the frontal region in the two cases of low or high M , respectively. In either case, the pressure drop is associated with the higher flow resistance. In the first case, it is due to the invading phase, which near the front occupies a percolation-like cluster. In the second case, it is due to the displaced phase, which near the front occupies a compact region. The different behavior in these two limits is the origin of the difference in the scaling exponents in the two limits. Such distinction was made by Lenormand [95], but not by Wilkinson [87] or Blunt et al. [96]. This explains why our exponent agrees with Wilkinson's only in the first limit case, but not in the second, where instead we agree with Lenormand. The difference between our exponent and Lenormand's [95] for the case of low M , was alluded to before and is due to the fact that in his calculation, Lenormand [95] used the entire injection rate Q , while here we assumed that only a small fraction of Q actually reaches the frontal region. This difference is ultimately reflected in the scaling exponents. We must point out, however, that Lenormand's assumption is correct for the specific problem he considered, which is the evaluation of the onset of the departure from percolation in a displacement in a square lattice, where travelling fronts and gradient percolation concepts are not involved. For the case of high M , where a correction for Q_w is not required, our exponent is identical to his.

4.3 Experiments

The VGP theory at small M was partially tested by conducting some experiments and pore network simulations. Immiscible displacement experiments were conducted in a long sample, consisting of a vertically placed rectangular glass bead pack of dimensions $30 \times 4 \times 2$ cm³, filled with 100 μ m glass beads, with porosity and permeability equal to $\sim 40\%$ and $\sim 40 \times 10^{-12}$ m², respectively. Gravitational effects were avoided by using matched-density fluids ($\rho = 1.15 \times 10^3$ kgm⁻³, $\delta\rho < 10$ kgm⁻³). Water-sucrose mixture was used as the wetting fluid ($\mu_w = 5 \times 10^{-3}$ Pa·s) and dibutyl phtalate was used as the non-wetting fluid ($\mu_o = 14 \times 10^{-3}$ Pa·s), resulting into a viscosity ratio of $M = 0.3$. The interfacial tension between the fluids was $\gamma \sim 25 \times 10^{-3}$ Jm⁻².

Experiments corresponded to primary drainage and involved the displacement of the wetting fluid from an initially water-sucrose-saturated sample by the non-wetting fluid. The flow rate q varied between 10^{-6} and 10^{-4} m/s, corresponding to a capillary number variation in

the interval between 5×10^{-7} and 5×10^{-5} . An acoustic technique, described elsewhere [110], was used to determine the saturation profile. Saturation measurements were indirectly obtained from the velocity variations of a sound wave along the sample. From the calibration curve [110] and the accuracy of the relative velocity measurements (10^{-4}) we estimate the overall accuracy in saturation as better than 1%. A spatial resolution of 1 mm was implemented in order to keep track of precise variations along the length of the sample.

Fig. 66 shows transversely-averaged profiles of the saturation of the non-wetting phase, S_{nw} , near the front, plotted vs the reduced sample length $X = x/L$ for two different flow rates. The figure shows the existence of a bent knee at the leading edge of the front, where saturations are generally small. At larger capillary number, the “knee” merges into the straight front. In the figure, the inset shows the full saturation profile. In general, the profile near the front has the general features of VGP described in Fig. 66, namely a slowly varying mean value and an extent that decreases as the capillary (or Bond) number increases. In addition, the upstream part of the profile varies over a smaller region, which is consistent with the different scaling with Ca of the continuum and VGP regimes described above. At sufficiently large rates, the knee merges into what we can describe as an almost sharp shock front. A log-log plot of the front extent vs capillary number is shown in Fig. 67. From the limited data available, the relationship appears to be a straight line, although there is some data scatter. The straight line of slope of -0.25 is the theoretical prediction, in good agreement with the data. Even though the agreement is good, additional experiments would be needed for a more rigorous test of the theory.

The theoretical predictions for the small M case were also tested with results from 2-D pore network simulations using the drainage network model described in Xu [102]. Simulations in a 40×100 network, with $M = 0.1$ and Ca varying in the interval between $Ca = 10^{-4}$ and 10^{-5} , showed a power-law scaling of the front width with the capillary number, with a best-fit slope of -0.34 (Fig. 68), in reasonable agreement with the expected value -0.382 [102]. Given the various finite-size effects due to the small sizes of the network, this agreement is somewhat surprising. A more stringent test should involve much larger lattices and much smaller Ca . Work in this direction is currently under way.

4.4 Remarks on the Effects of Heterogeneity

We conclude this paper by making some additional remarks on the validity of the continuum theory. The latter was based on the assumption that expressions, such as (45), are deterministic, namely that saturation gradients are sufficiently small for volume-averaged quantities to be statistically meaningful. To set a quantitative condition for the validity of this assumption we proceed as follows.

Consider a 3-D volume containing N_s occupied and uncorrelated pores with the statistics described before and define a volume-averaged quantity $\langle \Psi \rangle_{N_s}$ over this volume. In general, this quantity is a random variable with a deterministic mean and a standard deviation that, in the large N_s limit, scales as $\Sigma N_s^{-1/2}$, as dictated by the law of large numbers [111]. This property is shared by all volume-averaged quantities, such as pressure, permeability,

Figure 66: Experimental drainage saturation profiles near the front: (a) $Ca = 9 \times 10^{-6}$, (b) $Ca = 4.5 \times 10^{-6}$. The inset shows the full profiles.

Figure 67: Plot of the front width vs. Ca from experimental results. The dashed line is the theoretical prediction of slope -0.254.

Figure 68: Plot of the front width vs. Ca from pore-network simulations with $M = 0.1$ in a lattice of 60×100 . The best-fit slope of -0.34 compares reasonably well with the theoretical prediction of -0.384.

etc. The conventional continuum description above relies on the existence of deterministic volume averages, hence on the requirement that the standard deviation of the volume averages does not exceed a small positive number δ , namely that

$$N_s \geq \left(\frac{\Sigma}{\delta}\right)^2 \quad (79)$$

Condition (79) shows that as expected, more disordered media require a larger averaging volume, for the definition of meaningful averages. For quantities that depend on the saturation (such as relative permeabilities and capillary pressures), however, deterministic volume averages additionally require that saturations are spatially uniform, namely that the scaled saturation gradient in the volume-averaged region, $g = -dS_{nw}/dX$, is sufficiently small,

$$g \leq \frac{\epsilon}{N_s^{1/3}} \quad (80)$$

where ϵ is the allowed standard deviation of S_{nw} (e.g., of the order of 10^{-3}). In the continuum description above, g was shown to scale with Ca . The two inequalities can be combined to lead to the following condition for the validity of the continuum description

$$Ca \leq O\left(\epsilon\left(\frac{\delta}{\Sigma}\right)^{2/3}\right) \quad (81)$$

Typical displacements are usually conducted at $Ca = 10^{-6}$, which appears to be within the range defined by (81). However, it becomes more difficult for this condition to be satisfied as the disorder, Σ , increases. (A corresponding constraint can be also derived for the validity of the VGP theory, by requesting that the predicted front width is sufficiently large for scaling laws, such as (32), to be valid.)

The previous theory identified three length scales of relevance to drainage processes in uncorrelated random media: In dimensionless terms, they are proportional to L (the lateral extent), to $Ca_F^{-1/(1+\nu(D-1))}$ (case 1) or $Ca^{-1/(1+\nu)}$ (case 2), and to Ca^{-1} . Heterogeneity in the pore structure can enter either through gradients in the mean pore size (in which case the pore size becomes a non-stationary variable) or through stationary, but spatially correlated, pore sizes. In either case, its effect on the saturation profile depends on the magnitude of the appropriate length scale. In the case of pore size gradients, the heterogeneity Bond number [2], $B_k = -\frac{dr_m}{dx}$, introduces a corresponding length scale which is proportional to B_k^{-1} . Here, effects of heterogeneity can still be captured by continuum equations, as done by Yortsos and Chang [112], provided that all the relevant length scales discussed above are smaller than this scale, which would then impose upper bounds on Ca . In addition, use of volume-averaged quantities requires sufficiently weak heterogeneity, namely

$$B_k < \delta^{2/3} \quad (82)$$

In the opposite case, heterogeneity would interfere with the development of the saturation profile. This can still be handled with the previous approach, however. For example, in the

absence of viscous forces it is known that gradients in the mean pore size lead to a stable form of IPG, when $B_k > 0$, and with B_k in place of B , and to an unstable form of IPG (capillary fingering) in the opposite case [2]. Thus, when viscous forces are also considered, we can combine heterogeneity and viscous gradients in an *additive* operation, the resulting scaling with respect to Ca being now accordingly different.

Different considerations apply when the local pore size is stationary but spatially correlated, with a dimensionless correlation length, λ . Here, the previous theory is still applicable, provided that the corresponding viscous lengths exceed λ significantly. Otherwise, the displacement would be affected by the heterogeneity. Recent publications [113] have studied effects of spatial correlations (involving fractal statistics) on IP. The effect of gradients on displacements in such fields is recently explored in [113].

When, as result of increased Ca , conditions such as (81) are violated, many of the previous postulates, for example the concept of deterministic volume averages, become questionable. In this case, suitable alternatives to the above must be sought. One approach could involve defining area- (instead of volume) averages, transverse to the main direction of displacement, which can be meaningful, provided that the lateral extent is sufficiently large. Here, some form of IPG is also expected to be applicable, since the displacement remains a percolation process, but with a gradient in the percolation probability. Work in this direction is currently in progress.

4.5 Conclusions

In this paper, the effect of viscous forces on drainage displacements in porous media was studied. We recognized that the process, at least near the front, shares common aspects with IPG. When M is sufficiently small, for example, as expressed quantitatively by condition (65), the displacement can be modeled by a form of Gradient Percolation in a *stabilizing* gradient, involving a percolation probability profile in the form of a “double hump” at the front termed VGP. We developed the scaling of the front width and the saturation profile, in terms of the capillary number. The results generalize the theory of Gouyet et al. [84] to arbitrary exponents near the front. As the stabilized regime is described by the Buckley-Leverett equation, a constraint for its validity is also developed. In the opposite case, the displacement is described by Gradient Percolation in a *destabilizing* gradient and leads to capillary fingering. This regime is identified for the first time and differs from DLA, which also describes displacements at large M . Constraints for the validity of the two regimes were developed. Limited experimental and numerical results support the theory. The effect of heterogeneity is also discussed. The theory shows that at least in the regions considered, the conventional continuum approach should be used with caution near the front. Upper bound conditions on Ca for the validity of the continuum approach was also developed. Similar results are also expected for imbibition (displacement of a non-wetting phase), provided that injection rates are sufficiently high [1].

5 Asymptotic Regimes in Displacements in Random Porous Media

Zhengmin Yang

5.1 Introduction

Two different displacement regimes, the Vertical Equilibrium (*VE*) and the Dykstra-Parsons (*DP*) regimes, have been used to model displacements in porous media. Vertical equilibrium is a commonly made assumption to describe fluid displacement [114, 115, 116, 117]. (A more accurate terminology should be *Transverse Equilibrium (TE)*, which will be followed here, since gravity is actually not necessary for its application). The parameter $R_L = L/H(k_V/k_H)^{1/2}$ was suggested as the controlling factor for a system to approach *TE* [114], and was analytically shown to be so by Yortsos [116]. In this regime, because of the large aspect ratio, transverse (vertical) flow is extensive. The Dykstra-Parsons (*DP*) approach [118] is used to describe processes when there is no transverse flow (for example, in case of non-communicating layers). The use of either *TE* or *DP* leads to a considerable simplification due to a reduction in the number of primary variables, and facilitates the development of average models and scale-up. This reduction is of interest to coarse-gridding in reservoir simulation.

Although the two regimes have been used extensively, the range of their applicability remains unclear, and even confusing. This is particularly the case for unstable displacements and viscous fingering problems. It is one of the objectives of this chapter to delineate the region of validity of these two regimes. We proceed with an asymptotic analysis of the full problem in the two limits $R_L \gg 1$ and $R_L \ll 1$ and show that the *TE* and *DP* regimes are obtained in the respective limits. In both cases, the problem is reduced to the solution of a single integro-differential equation. For the *TE* case, the limit obtained is akin to the *lubrication* approximation in viscous flows [119]. To study the validity of these asymptotic approximations, we investigate the solution of the full problem using R_L as a parameter. In the full model, both pressure and concentration fields are solved. We use standard methods of High Resolution Solution (*HRS*) to study displacement patterns as well as the behavior of transverse averages in concentration and mobility, needed for the assessment and development of viscous fingering models. The analysis is for 2-D geometries and for the miscible problem only. Extension to other processes, including immiscible processes and gravity effects, is straightforward, but it will not be reported here.

The simulations show that the development of the *VF* patterns and the transverse averages depends on the parameter R_L , in addition to the mobility ratio M . Previous *VF* models, such as the Koval model, the Todd and Longstaff model and the Fayers model, do not account for such variation. However, the validation of these models is done using *HRS* or experimental results at a particular R_L value, usually $R_L = 3$. At the same time, a basic hypothesis in their derivation is the assumption of “parallel flow” implied in both limits dis-

cussed above. A connection to these regimes has not been established, with the exception of Waggoner [120], who also attempted to develop an empirical model that matches numerical simulations done at the TE limit. At present, none of the three empirical models can be derived in a self-consistent manner. It is the second objective of this chapter to proceed with an analysis of the equations at the TE limit, where VF persists, that lead to a more rigorous VF model. This model is based on the distinction between fingered and non-fingered regions and accounts for transverse mixing and for the variance of the mobility (and concentration) in the fingered zones. It is shown that this model adequately describes the main viscous features observed.

The chapter is organized as follows: First, we proceed with a mathematical description from which we derive in the two limits $R_L \gg 1$ and $R_L \ll 1$, the TE and DP approximations, respectively. Then, we use HRS to study the dependence of the patterns on R_L and show that the two asymptotic limits are consistent with the solution of the full problem. The last section deals with the derivation of a VF model based on the TE equations that includes the variance of the mobility inside the fingered region.

5.2 Mathematical Formulation

Consider miscible flow in a heterogeneous, but spatially uncorrelated, porous medium of a two-dimensional rectangular geometry. We proceed by assuming that the fluids are incompressible and first-contact miscible, and that mixing of fluids does not cause volume change. Based on these assumptions, the mathematical model is described by

$$\phi \frac{\partial c'}{\partial t'} + \frac{\partial(u'c')}{\partial x'} + \frac{\partial(v'c')}{\partial y'} = \nabla \cdot (D \nabla c) \quad (83)$$

$$u' = -\frac{K_H}{\mu'} \frac{\partial p'}{\partial x'} \quad (84)$$

$$v' = -\frac{K_V}{\mu'} \frac{\partial p'}{\partial y'} \quad (85)$$

$$\frac{\partial u'}{\partial x'} + \frac{\partial v'}{\partial y'} = 0 \quad (86)$$

where l stands for the real physical scale, ϕ is porosity, c is concentration of the injected fluid, u and v are longitudinal and transverse velocities, D is the dispersion coefficient, and K_H and K_V are longitudinal and transverse permeabilities, respectively.

The above system of equations can be nondimensionalized using the following dimensionless parameters: $K_H = k_h \kappa(x, y)$; $K_V = k_v \kappa(x, y)$; $\epsilon = \frac{H}{L}$; $x = \frac{x'}{L}$; $y = \frac{y'}{H}$; $c = \frac{c'}{c_0}$; $t = \frac{t'}{L/q}$; $u = \frac{u'}{q\phi}$; $v = \frac{v'}{q\phi}$; $\mu = \frac{\mu'}{\mu_0}$; $\lambda = \frac{1}{\mu}$; $\delta = \frac{k_v}{k_h}$; $p = \frac{p'}{Lq\phi\mu_0/k_h}$; $v = \epsilon w$; $N_{TD} = \frac{D}{\epsilon\phi qH}$; $R_L = \frac{\sqrt{\delta}}{\epsilon}$, to yield the following system of equations

$$\frac{\partial c}{\partial t} + \frac{\partial(uc)}{\partial x} + \frac{\partial(wc)}{\partial y} = N_{\parallel} \frac{\partial^2 c}{\partial x^2} + N_{\perp} \frac{\partial^2 c}{\partial y^2} \quad (87)$$

$$u = -\kappa\lambda \frac{\partial p}{\partial x} \quad (88)$$

$$\frac{1}{R_L^2} w = -\kappa\lambda \frac{\partial p}{\partial y} \quad (89)$$

$$\frac{\partial u}{\partial x} + \frac{\partial w}{\partial y} = 0 \quad (90)$$

Here we introduced the inverse *Peclet* numbers, $N_{\parallel} \equiv \frac{D_{\parallel}}{qL}$ and $N_{\perp} \equiv \frac{D_{\perp}L}{qH^2}$. If only molecular diffusion is considered, $N_{\parallel} = \epsilon N_{\perp}$, where $\epsilon \equiv \frac{H}{L}$ is the inverse of the geometric aspect ratio. The conventional initial and boundary conditions are: $c = 0$ at $t = 0$; $v = 0$ at $y = 0$ and $y = 1$; $\int_0^1 u dy = 1$, $v = 0$ (namely, $p = \text{const}(t)$) and $c - N_{\parallel} \frac{\partial c}{\partial x} = 1$ at $x = 0$; and $\frac{\partial c}{\partial x} = 0$ and $p = 0$ at $x = 1$. However, for reasons to be discussed below, we will also consider the solution of the problem subject to *periodic* boundary conditions at the boundaries $y = 0$ and $y = 1$.

The above formulation contains the dimensionless parameters $N_{\parallel}$, $N_{\perp}$, R_L^2 , the functional relation between mobility and concentration, and the two scale ratios $\frac{\Lambda_F}{L}$ and $\frac{\Lambda_V}{H}$ (the latter for the case of spatially varying permeabilities, where Λ_i denotes characteristic correlation lengths in the respective directions). Here, we focus only on displacements in uncorrelated fields of weak heterogeneity, where $\frac{\Lambda_F}{L}, \frac{\Lambda_V}{H} \ll 1$. As discussed above, the emphasis of the work is on the behavior of the system as a function of the modified aspect ratio, R_L . Note that in an isotropic medium, R_L reduces to the geometric aspect ratio, $R_L = \frac{L}{H}$, hence, large or small R_L effectively implies large or small aspect ratio, respectively.

5.2.1 Large R_L Limit.

Consider the asymptotic behavior of Eq.(89) in the limit $R_L \gg 1$ and take a regular asymptotic expansion of the dependent variables in terms of R_L^{-2} , such that

$$u = u_0 + \frac{1}{R_L^2} u_1 + \dots \quad (91)$$

$$w = w_0 + \frac{1}{R_L^2} w_1 + \dots \quad (92)$$

$$p = p_0 + \frac{1}{R_L^2} p_1 + \dots \quad (93)$$

$$c = c_0 + \frac{1}{R_L^2} c_1 + \dots \quad (94)$$

In the limit, $R_L \gg 1$, Yortsos [116] showed that $0 = \frac{\partial p_0}{\partial y}$ and the pressure variation is

$$\frac{\partial p_0}{\partial x} = -\frac{1}{\int_0^1 \kappa \lambda dy} \quad (95)$$

Under these conditions, the concentration evolves according to

$$\frac{\partial c}{\partial t} + \frac{\partial(uc)}{\partial x} + \frac{\partial(wc)}{\partial y} = N_{TD} \frac{\partial^2 c}{\partial y^2} \quad (96)$$

$$u = \frac{\kappa \lambda}{\int_0^1 \kappa \lambda dy} \quad (97)$$

$$w = -\frac{\partial}{\partial x} \left(\frac{\int_0^y \kappa \lambda dy}{\int_0^1 \kappa \lambda dy} \right) \quad (98)$$

where we omitted the subscript 0 for simplicity. It follows that in this limit, longitudinal and transverse velocities become explicitly related to mobility (concentration). It must be noted that although the pressure is to leading-order independent of the transverse coordinate y (hence the term *Vertical or Transverse Equilibrium*), there exists substantial transverse mixing, as the transverse velocity w is non-zero, in general. The transverse velocity could vanish in many cases, for example in tracer diffusion in a layered system, where $\lambda = 1$ and κ depends on y only. In such cases, the vanishing of the velocity has often led to confusing the *TE* with the *DP* regime, where the leading-order transverse velocity is by definition *nil* (see also below). A final substitution of (15) and (98) into (96) leads to a single integrodifferential equation for the concentration

$$\frac{\partial c}{\partial t} + \frac{\kappa \lambda}{\int_0^1 \kappa \lambda dy} \frac{\partial c}{\partial x} - \frac{\partial}{\partial x} \left(\frac{\int_0^y \kappa \lambda dy}{\int_0^1 \kappa \lambda dy} \right) \frac{\partial c}{\partial y} = N_{\parallel} \frac{\partial^2 c}{\partial x^2} + N_{\perp} \frac{\partial^2 c}{\partial y^2} \quad (99)$$

The problem, therefore, is reduced to the solution of the integrodifferential equation (99).

In the above, the use of no-flow boundary conditions at the lateral boundaries was implied. However, as discussed in Yang [121], this problem suffers at the *TE* limit from a boundary effect. To avoid this problem, we applied in the remainder periodic boundary conditions. In this case, the expression for u remains as in (15), however, the expression for the transverse velocity is modified to read (see Yang [121])

$$w = -\int_0^y \frac{\partial u}{\partial x} dy + \frac{\int_0^1 \frac{1}{\kappa \lambda} \int_0^y \frac{\partial u}{\partial x} dy' dy}{\int_0^1 \frac{1}{\kappa \lambda} dy} \quad (100)$$

All numerical solutions reported below are based on the use of such periodic boundary conditions.

5.2.2 Small R_L Limit.

The other asymptotic limit is obtained at small R_L . Expanding (90) using the asymptotic expansion

$$u = u_0 + R_L^2 u_1 + \dots \quad (101)$$

$$w = w_0 + R_L^2 w_1 + \dots \quad (102)$$

$$c = c_0 + R_L^2 c_1 + \dots \quad (103)$$

and taking the limit $R_L \rightarrow 0$, we obtain to leading order

$$w_0 = 0 \quad (104)$$

which when inserted in (89) shows that u_0 is x -independent. Using the appropriate boundary conditions, it is not difficult to derive the following expression for the streamwise velocity

$$u_0 = \frac{1}{\int_0^1 \frac{dx}{\kappa\lambda(c_0)} \int_0^1 \frac{dy}{\kappa\lambda(c_0)}} \quad (105)$$

The concentration field is now obtained as the solution of the following integrodifferential equation

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = N_{\parallel} \frac{\partial^2 c}{\partial x^2} + N_{\perp} \frac{\partial^2 c}{\partial y^2} \quad (106)$$

where subscript 0 was also omitted and u is given from (105) with the subscripts suppressed.

Equations (105) and (106) describe the Dykstra-Parsons limit. Comparison between (99) and (106) shows the difference in transverse flow in the two regimes: In the *TE* regime, transverse flow is significant and is driven by mobility or permeability variations. In the *DP* regime, transverse flow is nil. In both cases, the streamwise velocity is explicitly related to concentration and permeability. In the *DP* problem, it is only dependent on the transverse coordinate y (layer-dependent). In the *TE* regime, u depends on both x and y . In places, however, where c and κ are only y -dependent, then w also vanishes in the *TE* limit, which may lead to confusing *TE* with *DP* (where $w = 0$ at all times) (see Lake [114]). Even then, the two expressions for u are different. Finally, it is interesting to note that for a passive tracer in a layered system, the *TE* limit *coincides* exactly with the *DP* limit. This is also another source of confusion between the two limits.

5.3 Numerical Results

To study the properties of the asymptotic limits, a numerical solution of the full model was considered. Numerical simulations of unstable displacements have used various approaches, including finite-difference schemes [122], spectral methods [123] and methods based on simulation along characteristic directions or streamtubes [124, 125]. A major difficulty in using finite differences for such predominantly convective problems is numerical dispersion and numerical oscillations. Both these problems can be overcome by the Total Variation Diminishing (*TVD*) method with flux limiter [126], which is a dynamic weighting between lower- and higher-order difference schemes, depending on the local flow condition. This technique will be used here (see Yang [121] for details). For unstable displacements, instability was triggered by fluctuations either in permeability or in the inlet concentration, both of which resulted into similar characteristics for the patterns (Figures 5.3, 5.3). For this reason, in this chapter we report results obtained only from fluctuations in the permeability field with the Dykstra-Parsons coefficient $V_{DP} = 0.05$.

Figure 69: Concentration Profiles at $M = 10$ for Different R_L With the Instability Triggered by a Perturbation in Injection Conditions.

Figure 70: Concentration Profiles at $M = 10$ for Different R_L With the Instability Triggered by a Perturbation in Permeability Field.

As pointed out above, the enforcement of no-flow boundary condition at the lateral boundaries gives rise under certain conditions to an undesirable boundary effect, consisting of a pronounced finger propagating along the boundary. This was clearly seen in our simulations when viscous forces dominate and the system approaches TE in a weakly heterogeneous reservoir (small values of V_{DP}). As will be described elsewhere (Yang and Yortsos [127]), this effect results from the violation of the no-slip condition at the boundary due to the use of Darcy's law. It can be avoided by the use of periodic boundary conditions, and such an approach was taken in this chapter. Incidentally, it should be mentioned that most of the previous work on VF was done at conditions far from TE [128, 122] (typically, R_L is 3), where there is no significant boundary effect. Displacements at TE conditions have also been simulated [129], however, the results reported are for strong heterogeneity ($V_{DP} \geq 0.5$), where the boundary effect is minimized [121]. On the other hand, Waggoner et al. [130] reported results at the TE limit [130], where a clear boundary effect can be identified.

The effects of R_L and M on the viscous fingering features are shown in Figures 5.3-5.3, which show concentration and pressure profiles for different values of R_L at two different M . The results of finite R_L are obtained using the full model, which considers both pressure and concentration as variables. However, the results for the TE ($R_L \gg 1$) and the DP ($R_L \ll 1$) regimes are obtained from simulations based on the respective TE and DP models (17) and (24), which contain only concentration as the independent variable. In either, use of periodic boundary conditions at the lateral boundaries is made. In all simulations the same computational grid is used (typically 100×100). The figures show patterns at $t = 0.3$. Variations in R_L can be accomplished, for example, by varying the aspect ratio L/H , while keeping k_V/k_H constant. Therefore, the patterns in the figures with $R_L < 1$ must be *compressed*, while those with $R_L > 1$ must be *stretched* to reflect the actual pattern in physical space.

Figure 5.3 shows that as R_L increase above 1, the VF pattern is characterized by a constantly decreasing number of fingers, which however have a larger width and a decreasing concentration. This is attributed to the increased transverse mixing as R_L increases. The emergence of a few dominant fingers at larger values of R_L is consistent with previous works (Zimmerman and Homsy [123]) which show the coarsening of VF patterns as the process evolves. Viewed differently, this pattern reflects the fact that because of the large R_L value (large aspect ratio), there is sufficient time for the injected fluid to sample the transverse direction, resulting into large transverse mixing. The mixing zone appears to decrease slightly as TE conditions are approached. Comparison between the various patterns shows that the TE limit, as described by the single equation (99), is indeed the asymptotic approach of the solution of the full problem as R_L increases.

By contrast, as R_L decreases below 1, the number of fingers increases, although their width decreases and their concentration increases, reflecting tendencies opposite to the case of large R_L . These characteristics reflect the lack of transverse flow (and communication) between the fingers in this limit. Viewed differently, the DP limit corresponds to the early part of a displacement process, in which no time is given for the fluid to sample the transverse direction, hence mixing is negligible. The DP limit, described by equation (106), appears

Figure 71: Concentration Profiles at $M = 50$ for Different R_L .

to be the correct limit of the full problem as R_L tends to zero. It should be noted that because of the small disorder in permeability (small V_{DP}), the DP pattern practically shows no fingering characteristics (piston-like displacement), in contrast to its TE counterpart, which displays a persistent VF behavior.

Similar results are shown in Figure 5.3, where $M = 50$. The increased value of M is reflected well in the TE limit, but not in the $R_L < 1$ regime, which is practically the same as before.

Figures 5.3-5.3 show concentration and pressure profiles for $M = 10$, and $R_L = 10, 1$ and 0.01 , respectively. The concentration contours have the features described previously, namely that as R_L increases, the number of fingers decreases. The pressure profiles are quite interesting. At large R_L (Figure 5.3), the pressure is shown to be practically independent of the transverse direction in accordance with Eq.(99) of the TE limit, although small transverse pressure gradients are discernible near finger tips. The pressure field rapidly approaches TE conditions at a small distance downstream and upstream of the mixing zone (which can be estimated to be of the order of $\frac{1}{R_L}$). At $R_L = 1$ (Figure 5.3) the pressure profile is more variable and clearly departs from the TE prediction. Here, the influence of the mixing zone extends all the way to the end of the domain. Even more pronounced is the fluctuation in pressure in the small R_L case (Figure 5.3). Here, the profile has the characteristics corresponding to displacement in a structure of non-communicating layers. Compared to Figure 5.3, where the pressure profile has the characteristics corresponding to displacement in a homogeneous system, the difference is quite instructive.

These results indicate that when R_L is greater than about 10, the viscous fingering pattern practically converges to that of the TE model, where the pressure contours are approximately independent of the transverse direction. The validity of the TE approximation does not seem

Figure 72: Concentration and Pressure Contours for $M = 10$ and $R_L = 10$.

Figure 73: Concentration and Pressure Contours for $M = 10$ and $R_L = 1$.

Figure 74: Concentration and Pressure Contours for $M = 10$ and $R_L = 0.01$.

to depend significantly on the mobility, as long as the displacement is unstable. At small value of R_L , on the other hand, the fingering pattern is reasonably well described by the DP model, provided that R_L is less than about 0.1. Now the pressure profile depends only on the mobility variation in the transverse direction as in a layered formation. These results indicate that overall, the TE and DP approximations are accurate descriptions of the displacement in the respective limits.

5.4 Viscous Fingering Models

We used HRS to study the dependence of the transverse average $\bar{c}$ on the convective variable x/t for different values of the parameters. Figure 5.4 shows the variation of $\bar{c}$ for $t = 0.3$ and for different values of R_L . Figure 5.4 shows a corresponding plot for $R_L = 5$ and different times. Two features are noticeable: As R_L increases, the curves become steeper, the mixing zone length reducing somewhat. The numerical results do not actually collapse on a single curve, but they fluctuate around a mean curve (which is to be fitted by the empirical models). The stochastic element of this curve reflects the VF instability. Otherwise stated, the deterministic VF models must be viewed as relating the variation of the expected value of $\bar{C}$ to the convective variable x/t . This raises the possibility that the analysis of the data must also account for fluctuations and their moments (e.g. as in Welty and Gelhar [17]). Such an approach is considered below.

Figures 5.4, 5.4 and 5.4 show the matching of the Koval, Todd and Longstaff and Fayers models to 2-D HRS results at different R_L values. The models fit the results reasonably well when R_L is of order one (Figure 5.4). When R_L increases, however, a discrepancy arises due to the steep finger shape near the finger tip and the finger base, which cannot be captured

Figure 75: Variation of Transversely-Averaged Concentration vs. x/t , for Various Values of R_L .

by these models. In addition, the fluctuation intensity appears to increase. It is evident that R_L has an effect on the fingering patterns, hence on the 1-D VF model. (As an extreme example to prove this point, consider the small R_L (DP) limit, where the displacement is almost piston-like). However, such an effect is actually not represented in the existing VF models, none of which contains R_L . We note that a parallel flow concept is implied in all such models, but a connection to TE has not been established. One could assume that all these models actually pertain to TE (although their calibration is made at finite R_L). In fact, it can be shown that in theory, a convective model, namely one where variables depend only on x/t , is only possible in the limit $R_L \rightarrow \infty$.

The empirical models of Koval [131], Todd and Longstaff [132] and Fayers [133] are all based on a 1-D fractional flow description using a transversely averaged concentration,

$$\frac{\partial \bar{c}}{\partial t} + \frac{\partial F(\bar{c})}{\partial x} = 0 \quad (107)$$

where $\bar{c} = \int_0^1 c dy$, $F = F(\bar{c})$, and the different models have a different approximation for fractional flow. In both the Koval and the Todd and Longstaff models, the fractional flow function is defined as

$$F(\bar{c}) = \frac{\bar{c}}{\bar{c} + (1 - \bar{c})/M_e} \quad (108)$$

where the effective mobility ratio M_e is calculated by assuming the fixed concentration $c_{fk} = 0.22$ inside the finger, for the Koval model, and by the expression $M_e = (\frac{\mu_o}{\mu_s})^{1-\omega}$, for the Todd and Longstaff model. The parameter ω is determined empirically and it is typically

Figure 76: Comparison Between Koval, Todd-Longstaff and Fayers Models and 2-D *HRS* Results at $R_L = 1$.

Figure 77: Comparison Between Koval, Todd-Longstaff, Fayers Models and 2-D *HRS* Results at $R_L = 5$.

Figure 78: Comparison Between Koval, Todd-Longstaff, Fayers Models and 2-D *HRS* Results at the *TE* Condition.

found to be about 2/3 [132]. From Eqs. (25) and (108) lead to

$$\bar{c} = \frac{\sqrt{\frac{M_e}{x/t}} - 1}{M_e - 1} \quad (109)$$

The model of Fayers incorporates additional physics and has a fractional flow defined as

$$F(c) = \frac{\Lambda c_f}{\Lambda + (1 - \Lambda)\mu_f/\mu_o} \quad (110)$$

The finger width Λ is related to the concentration of the finger, C_f , by an ad-hoc expression [134]. For example, the following different forms have been proposed

$$\Lambda_1 = a + (1 - a)c_f^\alpha \quad (111)$$

$$\Lambda_2 = \frac{\mu_{fK} - \mu_f}{\mu_o - \mu_f - (\mu_o - \mu_{fK})c_f} \quad (112)$$

and

$$\Lambda_3 = c_f^{\beta/(1-\beta)} \quad (113)$$

where μ_{fK} is the viscosity inside a finger (as in Koval's model). The parameters in all these expressions are unspecified and must be determined by fitting with experimental or numerical results.

As discussed above, the derivation of a purely convective model is theoretically possible at conditions of *TE*. We proceed as follows: Consider the basic set of the *TE* equations

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} + w \frac{\partial c}{\partial y} = N_{\perp} \frac{\partial^2 c}{\partial y^2} + N_{\parallel} \frac{\partial^2 c}{\partial x^2} \quad (114)$$

$$u = \frac{\kappa \lambda}{\int_0^1 \kappa \lambda dy} \quad (115)$$

$$\frac{\partial u}{\partial x} + \frac{\partial w}{\partial y} = 0 \quad (116)$$

By multiplying by nc^{n-1} ($n = 1, 2, 3, \dots$) and integrating over y in the interval $[0, 1]$ we obtain a set of equations for the moments of c :

$$\begin{aligned} \frac{\partial}{\partial t} \left(\int_0^1 c^n dy \right) + \frac{\partial}{\partial x} \left(\frac{\int_0^1 \kappa \lambda c^n dy}{\int_0^1 \kappa \lambda dy} \right) \\ = -N_{\perp} n(n-1) \int_0^1 \left(\frac{\partial c}{\partial y} \right)^2 c^{n-2} dy \\ + N_{\parallel} \epsilon^2 n \int_0^1 c^{n-1} \frac{\partial^2 c}{\partial x^2} dy \end{aligned} \quad (117)$$

where we made use of the boundary conditions at the lateral boundaries. Equivalently, we may multiply Eq.(114) by $\dot{\lambda} = d\lambda/dc$ (assumed non-zero) to obtain

$$\frac{\partial \lambda}{\partial t} + u \frac{\partial \lambda}{\partial x} + w \frac{\partial \lambda}{\partial y} = N_{\perp} \dot{\lambda} \frac{\partial^2 C}{\partial y^2} \quad (118)$$

where we neglected longitudinal dispersion. We can construct moments of λ by multiplying by $n\lambda^{n-1}$ and integrating over y in the interval $(0, 1)$, as previously, to get

$$\begin{aligned} \frac{\partial}{\partial t} \left(\int_0^1 \lambda^n dy \right) + \frac{\partial}{\partial x} \left(\frac{\int_0^1 \kappa \lambda^{n+1} dy}{\int_0^1 \kappa \lambda dy} \right) \\ = -N_{\perp} \int_0^1 (\lambda^n)'' \left(\frac{\partial c}{\partial y} \right)^2 dy \end{aligned} \quad (119)$$

As in turbulent flow, further progress requires closure at some level. The first step is to distinguish between fingered and non-fingered regions (see Figure 5.4).

Assume that a fixed concentration $c_c \ll 1$ delineates the two regions and denote by $y_i(x, t)$ and $y_{i+1}(x, t)$ the boundaries of finger i . From now on, we let overbar denote averages *over the finger* region only, the overall width of which is Λ . For convenience, we define the normalized mobility

$$\lambda_f = \frac{\lambda - 1}{M - 1} \quad (120)$$

which varies in the interval $[0, 1]$. In this notation, λ_f is negligible outside the finger. The next step is to evaluate the various moments of λ_f in the finger region. We used the numerical

Figure 79: Definition of Mean Concentration Inside the Fingered Region.

solution for their estimates. Figures 5.4-5.4 show the variance $\sigma_\lambda^2 = \overline{\lambda_f - \bar{\lambda}_f}$ plotted vs. the mean value $\bar{\lambda}_f$ for different values of M . In all cases, the variance vanishes at the end points and reaches a maximum value somewhere in-between. To a good approximation, this maximum is nearly independent of M for the values tried and follows the best-fit expression

$$\sigma_\lambda^2 = \lambda^{1.8}(1 - \lambda)^{2.5} \quad (121)$$

Qualitatively, this behavior is expected, since the end-points correspond to the tip and base of the mixing zone, where all variability vanishes. Additional moments were also computed. Figure 5.4 shows higher-order moments for $M = 10$. It is shown that all higher moments are considerably smaller than the second, a result which is expected, in view of the definition of VF . This suggests that we can proceed with a small fluctuation approach. We should point out that a small perturbation analysis was also made by Welty and Gelhar [135], except that these authors did not differentiate between fingered and nonfingered regions. Because of the sharp changes in concentration and mobility across fingers, this approximation may not be adequate.

The importance of the second moment can be seen by considering the equation describing the first moment ($n = 1$ in (37)), which reads after appropriate manipulations

$$\begin{aligned} \frac{\partial}{\partial t} [\Lambda \bar{\lambda}_f] + \frac{\partial}{\partial x} \left[\frac{\Lambda [\bar{\lambda}_f + (M-1)\bar{\lambda}_f^2(1 + \frac{\sigma_\lambda^2}{\bar{\lambda}_f^2})]}{1 + (M-1)\Lambda \bar{\lambda}_f} \right] \\ = -N_\perp \int_0^1 \bar{\lambda}_f \left(\frac{\partial c}{\partial y} \right)^2 dy \end{aligned} \quad (122)$$

Figure 80: Mobility Variance vs. Normalized Average Mobility, λ_f (The Solid Line Denotes the Fit with the Expression (39)).

Figure 81: Mobility Variance from *HRS* Results (The Solid Line Denotes the Fit with the Expression (39) for Various Values of M).

Figure 82: Variation of Higher-Order Mobility Moments ($M = 10$, TE).

Comparing with Figures 5.4 and 5.4, we observe that although the ratio $\frac{\sigma_{\lambda}^2}{\bar{\lambda}_f}$ becomes small at value of $\bar{\lambda}_f$ near one, it cannot be neglected at smaller values of $\bar{\lambda}_f$ (which in fact dominate the VF behavior).

Further progress requires one additional equation for the evolution of the finger width Λ , the derivation of which will be discussed elsewhere. It can be shown that Λ satisfies

$$\frac{\partial \Lambda}{\partial t} + \frac{\partial}{\partial x} (\Lambda \bar{u}) = S \quad (123)$$

where S denotes transport between fingered and non-fingered regions. Yang [121] considered the particular case, where

$$S = \Lambda \frac{\partial \bar{u}}{\partial x} \quad (124)$$

Further analysis commenting on the validity of this and other related approximations will be reported elsewhere. Then, assuming a negligible RHS in Eq.(122), we obtain the system

$$\frac{\partial \Lambda}{\partial t} + \frac{1 + (M-1)\bar{\lambda}_f^*}{F} \frac{\partial \Lambda}{\partial x} = 0 \quad (125)$$

$$\frac{\partial (\Lambda \bar{\lambda}_f^*)}{\partial t} + \frac{\partial}{\partial x} \left[\frac{\Lambda \bar{\lambda}_f^* + (M-1)\Lambda \bar{\lambda}_f^{*2} + (M-1)\Lambda \sigma_{\lambda}^2}{F} \right] = 0 \quad (126)$$

where the variance is given by (39). The system is subject to the following initial and boundary conditions: $\Lambda(x, 0) = 0$, $\bar{\lambda}_f(x, 0) = 0$, $\Lambda(0, t) = 1$, $\bar{\lambda}_f(0, t) = 0$.

Figure 83: Comparison Between 2-D *HRS* Results and the *VF* Model for $M = 10$.

The above hyperbolic system can be solved both analytically and numerically. Numerical results are shown in Figure 5.4. It can be seen that the main *VF* features are well captured, especially the steep mobility shock in the finger base region, which neither of the previous models can capture adequately (Figure 5.4). The effect of M is shown in Figure 5.4. The model captures quite well the *VF* features for several values of M at *TE*. Further details can be found in Yang [121]. We should mention that Waggoner [17] also attempted the development of a similar *VF* model at *TE*. In our notation, his model is equivalent to setting $S = 0$ in (41) and $\sigma_\lambda^2 = 0$ in (44). Under these conditions, the solution of the hyperbolic system leads to a *VF* model which underpredicts the propagation speed of the base and overpredicts the propagation speed of the tip (which can be shown to be equal to $\frac{1}{M}$ and M , respectively). It appears that for a realistic model, careful consideration must be given to both S and σ_λ^2 . Further work in this direction will be reported elsewhere.

Figure 84: Comparison Between 2-D *HRS* Results and the *VF* Model for Different Values of M .

5.5 Discussions and Conclusions

In this chapter, we studied the asymptotic behavior of miscible displacements in porous media in the two limits, where a permeability-modified aspect ratio, $R_L = L/H(k_v/k_H)^{1/2}$, becomes large or small, respectively. The first limit is known as Vertical Equilibrium (*VE*), while the second leads to the Dykstra-Parsons (*DP*) problem. In either problem, we showed that the problem reduces to the solution of a single integro-differential equation. By comparison with *HRS* results, we showed the important effect of R_L , particularly for *VF* problems. For the latter case, we developed a *VF* model at the *TE* condition, which accounts for the variance of the mobility in the fingered zone, and for transport between “fingered and non-fingered” zones. The model appears to capture correctly the main features of the simulation.

6 Invasion Percolation and Gradient Percolation in Correlated Pore Networks

Chang-An Du and Y. C. Yortsos

6.1 Introduction

In this chapter we focus on the features of *IP* in lattices which are correlated. We begin with a brief introduction. Percolation properties, especially the percolation threshold find important applications in the physical processes. In addition, we discuss processes involving *Percolation in a Gradient* in such lattices. The latter process also finds important applications in petroleum, chemical engineering and porous media studies, particularly in the presence of gravity, viscous, or permeability gradients.

We know that many applications of engineering interest involve spatially correlated properties obeying the statistics of *fractional Brownian motion* (*fBm*)^[136]. Because of its spatially growing correlations^[137], *fBm* is a special, but important example of spatial correlation. In applications related to chemical engineering, *fBm* statistics have been shown to describe: pressure fluctuations in a bubble column^[138] or solid-liquid fluidized beds^{[139][140]}; the surface morphology of fracture surfaces, such as poly(styrene) and poly(methyl methacrylate)^[141] and more generally of rough substrates^[142]; the pore surface of various porous media^[143]; and the trace of propagating cracks^[144]. *fBm* was also conjectured to describe the distribution of permeabilities in various oil reservoirs^[145], in an attempt to explain field data of Arya et al.^[146], which indicated spatially growing correlations. In fact, the so-called *fractal geostatistics* have been successfully used in various practical situations (e.g. see Emmanuel et al.^[147]).

There are two applications where percolation processes in a field described by *fBm* may arise: The immiscible displacement of one fluid by another in a 2-D fracture, the aperture of which obeys *fBm* statistics; and the same displacement in a heterogeneous porous medium, the permeability of which obeys *fBm* statistics. In either case, it is assumed that capillary forces dominate the displacement. In previous works, Yortsos and Chang^[148] and van Batenburg et al.^[149] simulated displacements in such fields, by considering both capillary and viscous forces. Here, we consider the case where viscous forces are small (low flow rates). As capillary-controlled displacement is described by *Invasion Percolation* (*IP*) (Wilkinson and Willemsen^[150], see also recent up-scaling to random permeabilities by Yortsos et al.^[151], 1993), the problem of interest is one of percolation in a correlated lattice.

Short-range correlations of the exponential, *Gaussian* and spherical models also find wide applications. Such models are more often cited in the mining, soil, water resources and petroleum reservoir literature. In some sense, all properties have short-range correlations. All three models stated above are similar, in the sense that they are short-range correlation

models, with their correlations decaying exponentially fast. For this reason, we only consider exponential correlation, a representative of such models. A typical exponential correlation has the form $C(r) \sim \exp(-r/\lambda)$, where r is the lag distance and λ the correlation length. Although exponential correlations are widely used, few studies discussed percolation. This may be because, in theory [152], exponential correlation is one of fast decay, where at large distances the correlation decays to zero, and above which, standard percolation applies with standard correlation exponents. Practically, of course, we may never have a sufficiently large system, but only finite systems of size L , which must be compared to the correlation length λ . In these problems two aspects need to be considered. The first is how a property changes with the system size L . Scale-dependent value such as percolation properties, and related conductivities, etc. could be derived. The second is how local, short-range correlations influence scale-up properties. For example, it is known that a local correlation length, λ , directly affects the longitudinal macro-dispersivity ($A_{11} = \sigma^2 \lambda / (1 + \sigma^2/6)^2$, where σ^2 is the variance of log permeability) [153], which can only be applied well in very large system ($L > 100 \times \lambda$). Apparently, the local correlation influence does not disappear in all systems and/or processes, as the system size increases.

Depending on the behavior of the correlation function at large values of the spatial lag, three cases of site percolation in a correlated lattice have been studied:

(i) When the decay is exponential, Renault [154] showed that the percolation threshold, p_c , of a correlated lattice is smaller than that of a random lattice (see also Ioannidis et al. [155] and also see below for more discussion.

(ii) When the correlation function decays algebraically, e.g. following $C(\rho) \sim \rho^{2H}$, $H < 0$, Prakash et al. [156] found that in site percolation in a square lattice, p_c decreases with increasing H , and approaches the value 0.5 at $H = 0$. For this problem, Isichenko [152] showed that the percolation exponent β , which scales the behavior of the percolation probability near p_c , remains the same as in the uncorrelated case. However, the correlation length exponent ν changes according to $\nu = -1/H$, $-0.75 < H < 0$. Using the relationship $D_f = E - \frac{\beta}{\nu}$, these results show that the fractal dimension D_f of the percolation cluster increases with H ($H < 0$), and approaches the embedding dimension $E = 2$ as $H \rightarrow 0$.

(iii) When the correlation function grows algebraically, as in an fBm lattice, where $H > 0$, Satik and Yortsos [157] reported, in an unpublished study of IP , that both the percolation threshold, p_c , and the percolation probability function, $P(p)$, are stochastic, different realizations resulting in different p_c values and different $P(p)$ curves. In particular, these curves did not converge to a universal curve with an increase in the lattice size, as is the case with OP in a random lattice. A theoretical understanding of this behavior can be provided by Isichenko [152], who analyzed 2-D OP in fBm lattices and proposed that the mass fractal dimension D_f is constant and equal to 2 (a compact cluster), although that of its perimeter, D_h , varies with H as $D_h = (10 - 3H)/7$. Schmittbuhl et al. [158] studied percolation in an fBm hierarchical lattice and showed analytically that the percolation threshold is indeed a *stochastic* variable with a *finite* variance. In contrast, Sahimi [159][160] reported deterministic percolation thresholds, which increase with H for $0 < H < 0.5$ and decrease for $0.5 < H < 1$,

and fractal percolation clusters with a fractal dimension equal to that of the random case, except for H near 1. In Schmittbuhl et al.^[158], however, the “percolation threshold” is expressed as the surface height not the open fraction. A systematic test of p_c on fBm field is one of the objectives of this chapter.

When the percolation process is in short-range correlated lattices, Renault^[154] found that p_c decreased when the correlation length increased, but reached a constant value of 0.5 when λ is sufficiently large (such as 5 for square) for 2D lattices regardless of lattice type. Further, he predicted that the percolation threshold for a 2D triangular bond network should increase from a value of $\sin(\pi/8)$ (0.347) to 1/2 for random to large λ correlated lattices, respectively. He found that for 3D cubic bond ($p_c = 0.25$), site (0.3116) and tetrahedral bond (~ 0.4) networks decay to a smaller value, $0.1 \sim 0.2$, when $\lambda > 3 \sim 5$ and claimed that p_c would converge to this range and keep constant for larger λ (the largest λ tested is 5). Ioannidis and Chatzis^[155] directly adopted Renault’s $\lambda = 5$ as a limit value for the correlation influence, assuming that beyond this correlation length, all different 3D networks would have identical percolation properties. They build a bond-site correlated network (site has exponential or *Gaussian* correlations and bond takes the minimum site radius between two adjacent pore radii) with a constant λ for site radius correlation and simulated the accessibility function, the capillary curve (which was found to be more gradually increasing than in an uncorrelated lattice) and the residual saturation (which was found to be less than in the uncorrelated lattice). They also claimed that in the correlated case, the percolation probability exponent β changed from 0.45 to 0.547. It is unclear why this value varies. In fact, we believe that in sufficiently large lattices, the exponent remains the same as in the uncorrelated case (in contrast to fBm fields). We also believe that Renault’s result of limit $\lambda = 5$ is inconsistent with the theory because we expect that when λ is large ($\lambda \gg r$), for a fixed network size the correlation will change to fBm type in view of the behavior $C(r) \sim \exp(-r/\lambda) \sim 1 - r/\lambda$ and $\gamma(r) \sim 1 - C(r) \sim r$, i.e., an fBm correlation with $H = 0.5$. Naturally, the short-range correlated field p_c testing is another objective of the study.

6.2 Percolation in Correlated Lattices

6.2.1 Percolation in an fBm Lattice

We consider site IP in an fBm 2-D square lattice, of sizes as large as 256×256 . Sizes were assigned to the sites following fBm statistics, using the method of *mid-point displacement and random addition* described by Voss^[161] (see also Feder^[137]) (see Appendix A for a brief review).

An invasion process (from top-to-bottom in Figure 85) was then simulated, using the standard rule that the front advances to the largest perimeter site, and applying no-flow conditions at the lateral sides. Snapshots of the displacement for different values of H are shown in Figure 85. As in Satik and Yortsos^[157], the invaded regions appear to be compact,

but with a fractal perimeter. Contrary to the random case, the features of the invading phase depend critically on the realization, which here can be simply changed by reversing the displacement (e.g. from bottom-to-top, from left-to-right, etc.), as can be also seen from a cursory inspection of the fBm field. From the data obtained, we calculated IP curves $P(p, H)$ for different realizations and H values. Here, $P(p, H)$ denotes the fraction of invaded sites, and as is conventional in IP , we defined $p = \int_{r_{min}}^{\infty} \alpha(r) dr$, where r_{min} is the *minimum* size of invaded sites and $\alpha(r)$ is the probability density function (pdf).

Figure 86 shows various $P(p, H)$ curves for $H = 0.5$, corresponding to different realizations. The following are noted:

1. Contrary to the random case, the curves are stochastic, different realizations for the same H giving rise to a different curve.
2. Because the invasion cluster is not fractal (see also below), these curves assume non-zero values much before “breakthrough” of the invading phase.
3. For a given realization, each curve consists of a succession of jumps, which is characteristic of Invasion Percolation (e.g. Roux and Guyon^[162]).

The frequency of the bursts decreases as H increases. These results are consistent with the earlier findings^[157] and with the theory of Schmittbuhl et al.^[158]. Certainly, universality in percolation properties does not apply in these systems, each invasion process being sensitive to the particular realization.

The percolation threshold, p_c , was studied by conducting a site OP process, using the cluster labeling algorithm of Hoshen and Kopelman^[163] (see also Stauffer and Aharony^[164]). It was found (Table 1) that p_c is a *random* variable, with a mean value $\langle p_c \rangle (H)$ that monotonically decreases with H , such that $\langle p_c \rangle (0) = 0.5$ (the value reached by Prakash et al.^[156] as H approaches zero from the negative side) and $\langle p_c \rangle (1) = 0.386$. Its standard deviation, $\sigma_p(H)$, is an increasing function of H , with $\sigma_p(0) \approx 0$ (the non-zero value due to finite size effects) and $\sigma_p(1) \approx 0.13$. These are consistent with Schmittbuhl et al.^[158].

Using these data, the density of the percolation cluster at p_c , $\rho(p_c, H) = \frac{P(p_c)}{L^2}$, was computed for various values of H and lattice sizes. The results, listed in Table 2, show that although a stochastic variable, $\rho(p_c, H)$ has mean and standard deviation practically independent of the lattice size, at least for large values of H . This should be contrasted to the random case, where the average density decreases with L , following the well-known power-law scaling $\rho \sim L^{-\beta/\nu}$, where $\beta = 5/36$ and $\nu = 4/3$. The lack of sensitivity to L (at least for larger H), confirms the observation that the percolation cluster is not fractal, in agreement with Isichenko’s (1992) argument ($\nu \rightarrow \infty$). It must be noted that the slow decrease for $H = 0.2$, shown in Table 2, most likely reflects finite size effects, which should disappear at larger L . Values of the perimeter fractal dimension D_h were also estimated and found in reasonable agreement with Isichenko’s (1992) prediction.

Next, we computed ensemble averages, $\mathcal{P}(p, H)$, by ensemble-averaging p for fixed P and H . The results are plotted in Figure 87 for different H values. The ensemble averages continuously deviate from the universal curve (random medium) as H increases, although there is some cross-over at large p . Lattice-size effects on the ensemble average curves were found to be negligible. As with p_c , the standard deviation was found to increase with H and

Figure 85: Consecutive snapshots of invasion at different values of the *Hurst* exponent H (0.2, 0.5 and 0.8) and invaded fraction P (0.2, 0.4, 0.6, 0.8) from top to bottom. Dark color denotes defending phase.

Figure 86: Invasion fraction curve $P(p, H)$ for $H = 0.5$ and different realizations.

	Lattice Size/Number of Realizations				
H	64x64/1000	128x128/500	256x256/100	512x512/100	1024x1024/100
1.00	0.3843 ± 0.1307	0.3817 ± 0.1274	0.3871 ± 0.1295	0.3864 ± 0.1291	0.3826 ± 0.1263
0.80	0.3944 ± 0.1247	0.3924 ± 0.1218	0.3986 ± 0.1240	0.3912 ± 0.1261	0.3944 ± 0.1196
0.65	0.4040 ± 0.1206	0.4030 ± 0.1182	0.4131 ± 0.1212	0.4103 ± 0.1212	0.4074 ± 0.1181
0.50	0.4180 ± 0.1164	0.4164 ± 0.1133	0.4269 ± 0.1153	0.4221 ± 0.1132	0.4204 ± 0.1137
0.35	0.4365 ± 0.1086	0.4335 ± 0.1060	0.4471 ± 0.1061	0.4431 ± 0.1030	0.4424 ± 0.1057
0.20	0.4876 ± 0.0802	0.4577 ± 0.0958	0.4646 ± 0.0931	0.4700 ± 0.0882	0.4647 ± 0.0875
0.00	0.4907 ± 0.0782	0.4931 ± 0.0740	0.4976 ± 0.0670	0.5038 ± 0.0673	0.5024 ± 0.0607
rand	0.5818 ± 0.0216	0.5872 ± 0.0121	0.5893 ± 0.0077	0.5908 ± 0.0044	0.5912 ± 0.0028

Table 1: Percolation Threshold, p_c , for Site Percolation in An fBm Lattice.

	Lattice Size/Number of Realizations				
H	64x64/1000	128x128/550	256x256/550	512x512/200	1024x1024/100
0.80	0.3583 ± 0.1263	0.3538 ± 0.1269	0.3555 ± 0.1277	0.3513 ± 0.1241	0.3485 ± 0.1099
0.50	0.3485 ± 0.1133	0.3425 ± 0.1136	0.3423 ± 0.1166	0.3364 ± 0.1120	0.3361 ± 0.1071
0.20	0.3298 ± 0.0985	0.3230 ± 0.0998	0.3185 ± 0.0999	0.3025 ± 0.0901	0.3004 ± 0.0838
rand	0.2563 ± 0.0748	0.2343 ± 0.0684	0.2215 ± 0.0674	0.2024 ± 0.0590	0.1854 ± 0.0548

Table 2: Density of the Percolation Cluster at Breakthrough, $\rho = P(p_c)/L^2$, for Site Percolation in An fBm Lattice.

to be larger as p decreases. A capillary pressure, $P_c \sim \frac{1}{r}$, was also computed, where r is the size of the site currently being invaded. For the random case, the plot of the capillary pressure vs. time (or saturation S of the invading fluid) has the noisy appearance of Figure 88a, the properties of which were analyzed by Roux and Guyon^[162]. For IP in an fBm lattice, curves corresponding to various H are shown in Figures 88b - 88d. The following two characteristics are noted:

1. Contrary to the random case, where it is flat, the envelope of P_c in the fBm case has a definite gradient, which increases with H .
2. The fluctuations diminish in size as H increases, reflecting the improved connectivity of the lattice, while the distribution of burst sizes is much narrower. The analysis of these bursts is currently under study.

6.2.2 Percolation in an Exponentially Correlated Lattice

We use a nearest-neighbor method to generate short range correlated lattices, see Appendix B for the model description. The resulting correlation is not exactly exponential, although its decay is. We found that when λ is not very large, the correlation is quite close to exponential. We also noticed that for a fixed α (which is the correlation degree parameter used in the nearest-neighbor model) the larger the lattice size, the stronger the correlation (larger correlation length estimated).

We varied both L and α to simulate various finite systems. Different values of α lead to different correlation lengths λ . Because of the large number of realizations needed, and the fact that evaluation of λ from a generated field each time is time-consuming, we used the approximation $\lambda = \sqrt{\frac{\alpha}{1-\alpha}}$ (see Appendix B) to indicate our correlation. During simulations, we first specify α , then, the nearest-neighbor model iterates to get a correlated field. Then we follow the same procedure as in fBm to calculate p_c . The results are shown in Table 3. The random case and $\alpha = 0.0$ (where the correlation between neighbors is zero) show the right trend, namely that p_c increases with the lattice size. For $\alpha = 0.4717$ ($\lambda = 0.9449$), p_c changes from 0.5162 for a lattice of 10×10 to 0.5694 for a lattice of 200×200 . We expect that for even larger lattice, p_c may actually go back to its random field value. For larger α (λ), p_c is indeed lower than 0.5. This shows the strong effect of local correlations (even $\lambda/L \sim 0.05$ is not very large). The lowest p_c values are quite close to the high H in the fBm case. This result confirms our previous argument. Namely, p_c for short range correlated fields should be scale-dependent.

In summary, in this section the results of both OP and IP in an fBm lattice show that the percolation threshold is not deterministic and decreases with H increase, supporting the results of Satik and Yortsos^[157] and the findings of Isichenko^[152] and Schmittbuhl et al.^[158]. The results of OP on nearest-neighbor generated lattice also show the scale-dependent nature of p_c on lattice size and correlation length. When the correlation length is large, for a fixed finite lattice, p_c reflects the fBm correlations. This result is consistent with the p_c value from the fBm lattice.

Figure 87: Ensemble average $\mathcal{P}(p, H)$ for different values of the *Hurst* exponent H (random, -0.5, -0.2, 0.0, 0.2, 0.5 and 1.0 from right to left).

Figure 88: Normalized capillary pressure curve vs. invasion time for different values of the *Hurst* exponent H and a fixed realization (a: random, b: 0.2, c: 0.5 and d: 0.8).

α	rand	0.0	0.4717	0.9346	0.9889	0.9972	0.9993	0.9998	0.9999
λ	rand	0.0	0.9449	3.7803	9.439	18.87	37.78	70.70	100
Size	p_c/σ_c								
10		0.5482	0.5162	0.4431	0.4003	0.3886	0.3860	0.3844	0.3879
#100		0.0688	0.0837	0.1148	0.1230	0.1174	0.1182	0.1154	0.1170
25	0.5745	0.5745	0.5456	0.4365	0.4164	0.3912	0.3796	0.3757	0.3748
#100	0.0350	0.0350	0.0474	0.0944	0.1006	0.1131	0.1159	0.1138	0.1180
50	0.5705	0.5705	0.5492	0.5031	0.4773	0.4610	0.4463	0.4278	
	0.0264		0.0264	0.0714	0.0993	0.1184	0.1221	0.1232	
#	50	50	50	20	20	50	50	50	
100	0.5881	0.5881	0.5593	0.5214	0.4678	0.4385	0.4051	0.3836	
#20	0.0141	0.0141	0.0190	0.0338	0.0923	0.1181	0.1375	0.1212	
200	0.5921		0.5694	0.5227	0.4853	0.4532			
#20	0.0099		0.0114	0.0284	0.0638	0.0787			

Table 3: Percolation Threshold ($p_c \pm \sigma_c$) vs Exponential Correlation Length λ .

6.3 Invasion Percolation in a Gradient

6.3.1 Introduction

Displacements in porous media at small rates (low values of the capillary number) are well described by invasion percolation (*IP*)^[165]. For statistically homogeneous uncorrelated random media, the displacement pattern is described by *IP* when capillary forces dominate and standard ordinary percolation properties including the critical exponents apply. In such cases, the interface forms a self-similar fractal^[137] with a specific fractal dimension. Because of the interesting percolation properties, slow drainage in porous media has attracted significant attention. At high injection rates, drainage is viscous-dominated, and for example leads to fingering, modeled by diffusion-limited aggregation (*DLA*^{[166][167]}), in the limit of large viscosity-ratio. At intermediate values of the capillary number, displacement process can be modeled by *GP* (gradient percolation) and *IPG* (invasion percolation in a gradient), which are modified versions of ordinary and invasion percolation respectively. Variations of the problem include diffusion, concentration gradients and permeability gradients^{[168][169][170][171][172][173][174][175][176]}. For example, in a 3D vertical displacement involving fluids of different densities, gravity forces compete with capillary forces. The dimensionless parameter $B_g = \Delta\rho g \bar{r}^2 / \gamma$, known as gravity or Bond number, measures the competition between gravity-induced hydrostatic and capillary forces, where g is the acceleration of gravity, $\bar{r}$, is the mean pore size, $\Delta\rho$ is the density difference and γ is the interfacial tension. If a light fluid is injected at the top of a heavy fluid, gravity will help to stabilize the displacement process ($B_g > 0$). Otherwise ($B_g < 0$), it will lead to unstable gravity

fingering. In the stable case, gravity acts to limit the front regime to a finite extent, in which case the front becomes self-affine. A compact region follows behind the front. In problems involving gradients in the percolation probability, the front extent is measured by the front width σ in two dimensions (2D) and by front-tail width σ_{FT} in three dimensions (3D). They both obey the following scaling law with Bond number:

$$\sigma \sim B_g^{-\frac{\nu}{\nu+1}} \quad (127)$$

where B_g is Bond number and ν the correlation length exponent of a percolation cluster. Thus, the effect of gravity for the stable case ($B_g > 0$) has been modeled with *GP* and *IPG*^{[177][172][174]}. This approach has been verified experimentally. Birovljev et al.^[178] confirmed the front width scaling law in 2D and found the predicted external perimeter exponent in the case of trapping. Clement et al.^[179] performed 3D *IP* experiments in the presence of gravity and determined the front hull fractal dimension from the front position statistics. Chaouche et al.^[175] also confirmed this scaling law in 3D experiments. Another extension of *GP* involves permeability gradients. Chaouche et al.^[175] modeled drainage in a permeability gradient using *IPG*. Because, however, the permeability gradient introduces a non-uniform pore space, a stretching of the real lattice was necessary.

Although much work has been done on the application of percolation to slow drainage, *GP* or *IPG* processes on correlated lattices have not been considered (although Sapoval et al.^[168] mentioned that the correlation between particles may play a role in the structure of the front). Because many realistic processes involve percolation in a gradient (e.g. due to gravity or viscous forces) in correlated lattices, which represent the majority of real media, we will also study in this chapter, invasion percolation in a gradient (*IPG*) in a short-range correlated field due to nearest-neighbor correlations and in long-range correlated fields using *fractional Gaussian noise (fGn)* and *fractional Brownian motion (fBm)*. The correlated pore network lattices considered can also be viewed as representing correlated permeability fields. We are particularly interested in determining how relation (127) changes for the case of correlated porous media. The results are compared to our studies of *OP* and *IP* in a correlated medium in the absence of gradients.

6.3.2 Theory

We recall that *GP* is a lattice percolation process, where the occupation probability p is not constant, but decreases (typically linearly) with one of the lattice coordinates^[168]. *IPG* is the analog of this process for invasion percolation. In the work of Sapoval^[168], the percolation probability $p(x)$ is spatially varying externally. In the work of Chaouche et al.^[175], the variation of p is related to that of the capillary pressure Π . The latter is the difference between the pressure of the non-wetting and wetting fluids across an interface at a pore throat of size r , where

$$\Pi = 2\gamma/r \quad (128)$$

The percolation probability is indirectly related to Π through

$$p = \int_r^\infty \alpha(r) dr \quad (129)$$

where $\alpha(r)$ is the pore size distribution.

In the absence of gradients, slow drainage is described by *IP*, where p is uniform in space, the front is a self-similar fractal, the correlation length obeys the scaling $\xi = |p - p_c|^{-\nu}$, and $\nu = 4/3$ or 0.88 in 2D or 3D, respectively.

In the presence of gradients, $p(x)$ is continuously decreasing (for the stable case) and the process is described by *IPG*. The front location x_c is identified from the condition $p(x_c) = p_c$. Evidently, the front location x_c varies with time, following a change with time of the imposed pressure $P(t)$. The vicinity of x_c is a crossover region, described by the theory of finite size effects in percolation^[137]. In both *GP* and *IPG*, there is a region around x_c of a finite extent σ , where percolation theory applies. Following Sapoal et al.^[168], the front position is defined as

$$x_f = \int_0^\infty x p(x) dx / \int_0^\infty p(x) dx \quad (130)$$

where x is the abscissa occupied by a particle of the front. In 2D, the definition of the front width is

$$\sigma^2 = \int_0^\infty (x - x_f)^2 p_f(x) dx / \int_0^\infty p_f(x) dx \quad (131)$$

The scaling of σ with the applied gradient is given by [168][171][177]

$$\frac{\sigma}{l} \sim |\Delta p|^{-\nu/(1+\nu)} \quad (132)$$

The same expression applies in 3D except that σ now denotes the front-tail width^[171], σ_{FT} . The saturation profile for the stable case^{[171][172]} is given from another scaling relationship

$$S \sim \frac{1}{K} \Pi_f \left[\frac{x_c - x}{\sigma} \right] \quad (133)$$

where K relates S of *IPG* to $p'_f = p_f/p$ of *GP* through $p'_f/(\delta p)^\beta = KS$ and $(p - p_c)/\delta p = (x_c - x)/\sigma$, $\delta p \equiv |\Delta p|^{1/(1+\nu)}$, $\beta = 0.14$ in 2D and 0.45 in 3D. Expressions for Π_f can be found in [171].

Consider now the application of the above to a permeability heterogeneity. Assuming a uniform size distribution $\alpha(r)$ of width b , and mean $\bar{r}$, then $p = (\bar{r} - r)/b + \frac{1}{2}$. Thus

$$\frac{dp}{dx} = \frac{1}{b} \frac{d\bar{r}}{dx} = -\frac{1}{b} B_k \quad (134)$$

where $B_k \equiv -d\bar{r}/dx \sim -d(\sqrt{k})/dx$. Proceeding as above, it is not difficult to show that

$$\frac{\sigma}{l} \sim B_k^{-\nu/(1+\nu)} \quad (135)$$

This equation is for random, uncorrelated porous media. Consider, now, the application to correlated media.

According to [152], for correlated porous media, the percolation correlation length exponent varies as

$$\bar{\nu} = -1/H \quad (136)$$

where $H(< 0)$ is the *Hurst* exponent for the *fGn* correlation function. Thus, to obtain the corresponding *IPG* in such correlated media, we substitute ν with $\bar{\nu}$ in equation (136) to get

$$\frac{\sigma}{l} \sim B^{-1/(1-H)} \quad (137)$$

This equation shows that the long-range correlation structure affects decisively the scaling exponent, and approaches -1 as the degree of correlation (or H) increases.

When the field becomes *fBm* correlated, with $H > 0$, Isichenko shows that $\bar{\nu} \sim \infty$. Direct application of the theory in this limit would indicate then a classical behavior (exponent -1),

$$\frac{\sigma}{l} \sim B^{-1} \quad (138)$$

According to this result, the scaling of the front width should be independent of the particular value of the *Hurst* exponent, H .

Finally, consider short-range correlated fields. Take for simplicity, the correlation function to be exponential, $\exp(-r/\lambda)$, where λ is the correlation length and r is the lag distance. When $\sigma \gg \lambda$, the correlation decays very fast within the front, hence we expect that the scaling would follow the random, uncorrelated front width equation (127), provided that the above constraint, $\sigma \gg \lambda$, applies. For example, this would be the case for sufficiently small B . In the other limit, $\sigma \ll \lambda$, the correlation within the region is strong. Consider the series expansion

$$\rho(r) = \exp(-r/\lambda) = 1 - \frac{r}{\lambda} + \frac{1}{2!} \left(\frac{r}{\lambda}\right)^2 + \dots \quad (139)$$

which, for sufficiently large λ , can be truncated to yield the following semi-variogram

$$\gamma(r) = 1 - \rho(r) \approx \frac{r}{\lambda} \quad (140)$$

In other words, we expect that the scaling would be the same as that of an *fBm* correlation function, $\gamma(r) \sim r^{2H}$, but with $H = 0.5$. In such cases, the correlation near the front would show a high *fBm* correlation and the front width should follow the scaling $\sigma \sim B^{-1}$. Between the above two extremes, there should be a transition zone, where we expect the exponent to vary from $\nu/(1+\nu)$ to 1. In summary, we expect that the initial part of the curve corresponding to high B_g , where σ is predicted to be small, would have slope of -1, characteristic of correlated *fBm* signals, while the latter part of the curve corresponding to lower B_g and higher σ would eventually display a slope of $-\nu/(1+\nu)$. Results are presented in the following section.

H	random	-0.8	-0.5	-0.2	0.0	0.2	0.5	0.8
Theory	0.57	0.57	0.67	0.83	1.00	1.00	1.00	1.00
Fitted	0.57	0.60	0.65	0.74	0.84	0.91	0.99	1.02

Table 4: The scaling exponent of the front width vs Bond number: theoretical and simulation values for 2-D fGn and fBm Correlated Fields.

6.3.3 Simulations and Discussion

(i) fGn and fBm correlated fields.

We used an fBm generator described in Appendix A to obtain different correlated fields with a different input value of H . As shown by Schmittbuhl et al.[158] the input value can be tuned to a negative value to simulate an fGn correlation function ($cov(r) \sim r^{2H}$ with $H < 0$). The fBm fields were normalized to $[0, 1]$. Subsequently, an IPG with gradient was applied. To do so, we selected a specific direction, e.g., direction j as that of the gradient, and assigned a spatially varying mean pore size following $\bar{r}(j) = -B(j - M)$, where $B > 0$, M is the lattice size in the j direction and j varies from 1 to M . Then, at a fixed value of j , we assigned pore sizes to all points in the perpendicular to j direction, $r(j, i) = fBm(j, i) + \bar{r}(j)$, $i = 1, 2, \dots, M$. A square lattice was used.

Before proceeding, we first tested this methodology using random fields. As shown in Figure 89, the slope in the scaling relation of the front width with the Bond number is perfectly matched with the theoretical value 0.571. Subsequently, we applied IPG in fGn and fBm correlated lattice. For the specific values $H = -0.8, -0.5, -0.2, 0.0, 0.2, 0.5$ and 0.8 , the results are also shown in Figure 89. The corresponding fitted slopes and theoretical values are also listed in Table 4. In general, the estimated slope is close to the theoretical values. The exception is the range $-0.2 \leq H \leq 0.2$, where there exist some differences. This may reflect the fact that the underlying lattice does not have sufficiently high correlations, perhaps due to finite size effect. Nonetheless, the straight line fitting two decades of B values show the correct power law correlation with an exponent of $\nu/(\nu + 1) = 1/(1 - H)$.

We must point out that during the simulations we found very strong size effects on the value of the front width especially at large H values and small Bond numbers. The front width increases with lattice size, everything else being fixed, until some limiting size is reached, where the width stabilizes. For small B value, this limit is quite large. Thus, in order to get accurate data we must use large networks for large H and small B . These size effects are shown in Figure 90 - 92. Figure 90 shows how σ changes with both lattice size and Bond number for $H = 0.8$. Figure 91 shows that under the conditions $H = 0.8$ and $B = 0.025$, the value of σ stabilized when the lattice size approached 256. However, Figure 92 shows that when $H = 0.8$ and $B = 0.001$, even a size of 1024 is not sufficiently large for σ to be stabilized.

Figure 89: Scaling of the front width σ vs the Bond number B for IPG in 2D lattices. The dotted line is the random case, where the fitted slope is -0.5724 . The solid lines from bottom to top correspond to fGn and fBm fields with $H = -0.8, -0.5, -0.2, 0.0, 0.2, 0.5, 0.8$, respectively. The fitted slopes are $-0.5978, -0.6494, -0.7389, -0.8396, -0.9112, -0.9919, -1.017$ respectively.

Figure 90: Scaling of the front width σ vs the Bond number B for *IPG* in 2D *fBm* lattice with $H = 0.8$. Both the lattice size and the Bond number B influence the front width σ . The numbers 128, 256, 512 and 1024 indicate lattice sizes. The asymptotic slope for the size 1024x1024 is 1.017.

Figure 91: Front width, σ , vs front position x_c for various lattice sizes with fixed Bond number $B=0.025$ in 2D fBm lattice with $H = 0.8$. The numbers 16, 32, 64, 128, 256 indicate lattice sizes.

Figure 92: Front width, σ , vs front position x_c for various lattice sizes with fixed Bond number $B=0.001$ in 2D fBm lattice with $H = 0.8$. The numbers 64, 128, 256, 512, and 1024 indicate lattice sizes.

(ii) Short-Range Correlated Field - Nearest-Neighbor Correlations.

Next, we used the nearest-neighbor correlation generator described in Appendix B to obtain fields correlated with different degrees. Similar to the fBm case, the field generated was normalized to $[0, 1]$ and then a given gradient was applied. The following α values, 0.5, 0.85, 0.95, 0.995, 0.999 were used to generate different correlation lengths. Note that as α increases, the correlation length also increases. Following the construction of the field, we conducted invasion percolation and calculated the corresponding properties. A size effect also existed in this case, i.e. for larger α (larger $\bar{\lambda}$), a larger size is needed to get σ values which are stabilized. Except for $\alpha = 0.5$, where a size of 400×400 was used, we used 1000×1000 lattices in all other cases. The results are shown in Figure 93. When $\alpha = 0.5$ ($\bar{\lambda} = 0.84$), the correlation is small, and the slope of the front width is very close to that of the uncorrelated random case. When the correlation length increases, the front width slope begins to show the theoretically predicted asymptotic slopes in the two regions, varying from a high value at small front widths to a low value at large front widths. The low slope value is close to that of the random case, namely, 0.571. The high slope region approximately extends over a distance corresponding to the correlation length scale, $\bar{\lambda}$. This high slope value increases when the correlation becomes stronger. Figure 93 shows that with a correlation length of $\bar{\lambda} = 3.178$, the high slope value of 0.88 exceeds the value of 0.84, which corresponds to an fBm with $H = 0.0$. This shows that the high slope region has a high correlation of the fBm type even though the nature of our correlated field is local. When the field has a correlation length of 20.02, the high slope reaches a value as high as 0.97 which corresponds to a very high H in the case of an fBm field. As we expected, when the correlation length $\bar{\lambda}$ is large, the high slope region is large, the transition period also increases and the low slope corresponding to the uncorrelated case does not appear in these simulations of a fixed network size.

6.4 Conclusions

In this chapter we tested percolation on correlated lattices of fBm and short-range correlations. The results of both OP and IP in an fBm lattice support the results of Satik and Yortsos^[157] and the findings of Isichenko^[152] and Schmittbuhl et al.^[158]. The statistics of the random variables p_c and $P(p, H)$ obtained should be useful in problems involving fBm lattices. More generally, the results should be useful in the study of invasion processes in correlated media. The results of OP on nearest-neighbor model generated lattice show the scale-dependent nature of p_c on lattice size and correlation length. When the correlation length is large, for a fixed finite lattice, p_c reflects the fBm correlations. This result is consistent with p_c value from fBm lattice.

We further conducted IPG on these correlated lattices. IPG can be used to describe slow drainage in the presence of gradients (gradient, viscous, permeability, etc.) in these fields. The theoretical analysis was confirmed by simulation. When the correlated field exhibits fGn long-range correlation, the front width scaling has the form $\sigma \sim B^{-1/(1-H)}$, namely the scaling exponent depends on the *Hurst* exponent H ($H < 0$). For fBm correlated

Figure 93: Scaling of the front width σ vs the Bond number B in 2D nearest-neighbor correlated lattices. The different curve from bottom to top correspond to $\alpha=0.5, 0.85, 0.95, 0.995$ and 0.999 with $\bar{\lambda}=0.8406, 1.745, 3.178, 9.6$ and 20.02 respectively. For $\alpha=0.5$, the curve is fitted by a single straight line of slope 0.593 ; for $\alpha=0.85$ and 0.95 , there are two limiting straight line segments, with slopes of 0.7784 and 0.88 , and 0.5912 and 0.5966 , respectively; for $\alpha=0.995$ and 0.999 , the curves can be fitted with straight lines at the early part (large B and small σ) with slopes of 0.9218 and 0.9715 respectively.

fields, on the other hand, the scaling is of the form $\sigma \sim B^{-1}$, namely the scaling exponent is constant and equals to one. Finally, for a locally correlated field, where the correlation function decays faster than algebraically, the front width scaling law has a variable exponent. Asymptotically, we can distinguish two limiting regimes: one at larger B and smaller σ , where, for sufficiently large λ , the exponent is equal to -1; and one at smaller B and larger σ , where the exponent approaches the value $-\frac{\nu}{1+\nu}$. Thus, the slope varies from an fBm -type correlation to that of random correlation case, as B decreases. In general, the large slope reflects the high correlation in short range. This region has a scale approximately equal to the lattice correlation length. When the lattice correlation length is larger than several lattice units, the large slope shows fBm -type correlations. In the range of $\sigma \gg \bar{\lambda}$, the other asymptotic slope is close to the uncorrelated value of $\nu/(1 + \nu)$.

7 Pore Size Distribution by Mercury Porosimetry and Percolation Theory

Chang-An Du and Y. C. Yortsos

7.1 Introduction

The porous media structure, namely, the distribution ($\alpha(r)$) of pore and throat sizes is very important in the study of fluid flow and reaction processes in porous media. A large number of efforts have been made on the study of the porous media structure. Two main models exist: capillary tube and network models. The capillary tube model is simple and easy to apply, and it has been traditionally used to interpret capillary pressure curves. A severe drawback of this model is that it does not account for the connectivity of pores and assumes that all pores are perfectly connected to the inlet and outlet. The interpreted curve distorts the real size distribution function: the middle size percentage is overestimated and that of the large size is underestimated. Network models, though more complicated, find more success in representing the real pore structure.

The primary probing tool employed in the study of porous media structure is mercury porosimetry

Mercury porosimetry, the forced intrusion of mercury into a porous material, has been used to characterize the porous media microstructure since Washburn^[180] suggested how to obtain a "pore size distribution" from a measurement of the volume injected vs. the applied pressure^{[181][182]}. Purcell^[182] introduced this technique to the petroleum industry^[183]. Since then, the capillary pressure P_c curves measured on reservoir rock samples (core, drilling cuts, chips etc.) have been used routinely in connection with petroleum research. The results obtained from this analysis relate petrophysical properties to the microstructure of reservoir rocks, e.g. for predicting permeability, relative permeability^{[184][185]}, resistivity, tortuosity, residual oil saturation, etc.^[186]. Mercury intrusion has also been used in other applications, for example to characterize activated carbon, adsorbent, porous catalysts, coal and coke, metal, ceramics, binding materials (such as cements, plasters), concrete, plastics, paper, textile, leather, wood etc.^[187].

In 1956, Fatt^{[188][189][190]}, made a very important contribution and introduced a network model to represent the porous media structure. Combined with the application of percolation theory^[191], the network models have become popular and powerful tool for the study of porous media structure. Although substantial progress has been made through network models and percolation theory for the understanding of porous media structure, a fully description of the pore structure is still unavailable. In [188], Fatt used 2D bond (zero volume of nodes) hexagonal, square, double hexagonal and triple hexagonal networks and simulated the capillary pressure curve and other properties. He studied the effect of lattice type, network size and bond size distribution. The results showed that both the lattice type

and the bond size distribution have effects on the capillary pressure curve. He used 200 to 400 bonds in each network simulation, but did not find apparent size effects. He then made corrections on the capillary tube model to interpret the bond size distribution from the capillary pressure curve.

Among many others^{[192][193][194][195][196][197][198]}, Diaz et al.^[199] considered a 3D cubic lattice with $z = 6$. In their model, pore body and pore throat both assumed slit shapes with Weibull distributions of the cross section sizes. The pore body size distribution was obtained from photomicrography, while the throat size distribution was obtained from mercury porosimetry (probably based on a capillary tube model). With this set of distribution parameters fixed, the authors tried to fit the simulated (by invasion percolation (*IP*)) capillary pressure with 10 sets of experiment P_c data. After 60% of non-wetting phase saturation, the simulated curve deviated from the experiment average curve. In another work, Chatzis and Dullient^[200] also used a cubic network of angular-shaped pore bodies and bonds, both with Beta functions, to simulate the capillary pressure curve and compared the results with 11 sets of experimental P_c data. The simulated curve deviated from the experimental average after $S_{nw} > 70\%$. More recently, the Matthews group^{[201][202][203]} presented a series of results based on network model simulations. Their network used to reproduce and/or model the P_c curve, porosity, tortuosity, connectivity, pore throat size distribution, gaseous diffusion through a dry sample, permeability and colloiddally induced formation damage. Their network model was a 10x10x10 cubic unit cell. Each node has z bonds on average with a cylindrical shape for each bond, and z is a random number varying from 0 to 6. Each node has a cubic shape and its size is the maximum surrounding bond diameter. They assumed a log linear bond size distribution of the form $\alpha(r) = \alpha(r_1) + k \log(r/r_1)$ with k , a normalization constant, determined from $\int_{r_1}^{r_2} \alpha(r) dr = 1$, where r_1 and r_2 were minimum and maximum bond sizes respectively. $\alpha(r_1)$ was a "skew" factor defined as being the percentage of throats of the smallest size in a log linear distribution. All pore bodies were centered at equal distance cubic lattice nodes. The distance between rows or columns of nodes, i.e., the bond length was adjusted by porosity requirement. Invasion percolation (*IP*) process was used to obtain the P_c curve. The saturation calculation considered a bond volume contribution. By minimizing the matching error between simulated and experimental P_c curves through the adjustment of the skew factor and z , they obtained the bond size distribution function and z at the same time. In our opinion, one of the important shortcomings of their model, is that the assumption of log-linear distribution is arbitrary and renders it no more than a traditional method. Also, important size effects (a difference between model and experiment core) were not addressed.

Observing that the usual pressure control mercury injection process can only give a bond size distribution (with the site saturation fraction not really a bond fraction), Yuan and Swason^[186] developed the method APEX ("Apparatus for Pore Examination") to conduct rate control mercury injection experiment with a very high resolution of $1 \times 10^{-6} \text{ cm}^3/\text{s}$ for the injection rate and 0.014kPa [0.002psi] for pressure to obtain both site and bond size distributions. Because of the high pressure resolution, the pressure fluctuations during pore and bond step-by-step penetration can be clearly recorded and displayed. They used the

term “subison” to refer to the region of increasing mercury pressure immediately following a rheon. In this region, the pressure was below the pressure at which the rheon occurred. “Rison” referred to the regions of increasing mercury pressure and corresponded to the filling of pore throats in such a way that all the mercury menisci changed uniformly. They counted the subison size as pore body volumes, transformed the volume data into size data and obtained the volume and/or size distribution. Following Yuan and Swanson^[186], Toledo et al.^{[204][205][206]} constructed a 3D network simulator to study the underlying mechanism. They used a randomized z to simulate a lattice with an average value different than 6. The node was assumed cubic and the connecting bond between two nodes was bi-conical. The minimum cross section size along the bond (middle point between two nodes) was taken as the bond size. The bond size (r_t) was drawn from a truncated log-normal distribution. The node size is the the maximum surrounding bond diameter multiplied by an aspect ratio, ρ , which is fixed for certain network, for example $\rho = 3.5$ and $\rho = 2.0$ for high (high porosity but poorly connected) and low (mimics consolidated sand stone) aspect ratios, respectively. The distance between rows of nodes or columns of nodes was fixed by porosity requirement. Through the volume and pressure constraints, the invading pores and pressure fluctuations can be solved. They obtained a similar pressure curve as in [186]. Their analysis showed that input bond and pore size distributions could be retrieved. When we consider a rate-control drainage process, the underlying principle is really very close to an invasion process. The only difference between this and the standard *IP* is that in this case, the continuous penetration of several bonds and pores during an avalanche event may need no apparent time to elapse, as the volume needed to fill the pore and bond volume deficit (because of constant and limited injection rate) is supplied by the withdrawing of all front pore interfaces, hence the deficit volume is gradually compensated by the injected volume. The pressure decreasing jump during the avalanche is also recovered by the injected volume. When pressure is recovered to the same (or higher than the previous) pressure, the total volume or time elapsed is the same as in standard *IP*. Thus, the envelope of the pressure curve is the same in both cases. We argue that the subison sizes must have some relation with the burst analysis of Roux and Guyon^[207], Gouyet^[208] and Maloy et al.^[209]. In the following, we will also review burst analysis and then analyze and conclude the work of [204].

Roux and Guyon^[207] analyzed all hierarchical burst (“subison”) sizes. They found a power law for the burst size distribution which relates to ordinary percolation exponents. Thinking that the burst analysis of [207] has no realistic time variable, Maloy et al.^[209] designed a 2D experiment and suggested a new invasion process to simulate the pressure jumps. The experiment was set up in a 120x175-mm transparent porous model with 1-mm glass beads packed between two plastic plates, with $\phi = 0.7$ and pore volume $\omega = 2\text{mm}^3$. The invading phase was air which displaced water at a constant rate $Q = 0.048\text{pores/s}$. Define $\Gamma = dp_{cap}/dt = dp_{cap}/dv * dv/dt = 1/K * Q/n_f$, where n_f is the number of pore throats in the front, $K^{-1} = dp_{cap}/dv$ and $dv = (Q/n_f)dt$. From the experiment data, $\Delta p(\Delta t)$ and $\Delta t * Q/n_f$, the parameter K could be estimated. That value was used in calculating the pressure steps. The key point in this experiment was that the porous media was loosely packed, hence, the pore radius was of the same size range as that of bonds. When one bond was

penetrated, with no need to further increase pressure, a bond surrounding the newly invaded pore was continuously selected and penetrated until the applied pressure could not overcome any other bonds. Because of the very low viscosity fluid (air), the pressure decreasing speed was so fast that no apparent time was needed to occupy multiple pores continuously (it acted like “jumps”). From these experiments, they offered the following analysis: In one pressure jump, multiple pores were occupied. These invaded pores were defined as a “burst”. Such “burst” is almost “half” the burst of Roux and Guyon^[207], because only the decreasing part was considered. They developed a new algorithm to simulate pressure jumps and the time intervals between jumps. As in *IP*, they found the $p_{i,min}$ among the bonds to be invaded. But in difference with *IP*, they also computed the time increment $dt = (p_{i,min} - p_{cap})n_f K$, where p_{cap} is the current capillary pressure (initially equal to 0) and $n_f \sim L^{D_c}$. Then the new time $t = t_0 + dt$ was calculated (initially $t_0 = 0$). After penetrating and invading events, a pore volume of V_i was occupied, the pressure decreased to $p_{cap} = p_{cap} - V_i/(n_f K)$ (at the first invasion, $p_{i,min} = p_{cap}$), and the process continued. The total pressure change in one burst is $\Pi = -\sum_i V_i/(n_f K)$. For $Kn_f \rightarrow \infty$, they proposed a scaling of the form $n(\Pi) = \Pi^{-\tilde{\tau}} f(\Pi/\Pi^*)(n_f K)^{(1-\tilde{\tau})}$ where $\Pi^* \sim (n_f K)^{-a}$, $f(x)$ is constant for $x \ll 1$ and approaches 0 at $x \rightarrow \infty$. These parameters are related to standard percolation exponents as in [207]. They found that both pressure jumps and buildup times (time steps between jumps) are exponentially distributed. Only in the limit $Kn_f \rightarrow \infty$ the dynamics are governed by power-law distributions.

Now, it is clear that Toledo et al.’s study is similar to Maloy et al.’s and in a certain aspect it is an invasion percolation process. The only difference is that the time intervals between jumps are collected in a hierarchical way in [209] and [207], while the volume interval in [204] is on the pressure envelope. In a sense, the volume interval should only have a relation with the invasion sequence which makes the burst size fixed. This “interval” of volume has no relation with the absolute pressure value. Then, we should guess that the size distribution from Toledo’s work follows an exponential or power law all the time with no relation to the underlying input distribution. Unfortunately, the truncated lognormal distribution looks like an exponential distribution, and we could not offer more judgment on their analysis. Actually other similar works were proposed of the resistance jumps analysis by Roux and Wilkinson^[210], Thompson et al.^[211], Batrouni et al.^[212] and Katz et al.^[213], where the cumulative size distribution of the resistance jumps was found to follow a power law. In conclusion, the pressure jumps and/or volume interval may not be applicable to derive pore size distributions.

More recently, percolation theory was introduced to interpret the capillary pressure curve^{[214][215][216]}. Mishra and Sharma^[217] used a Bethe lattice (pore throats and pore bodies) network in their *Monte Carlo* simulation study which lead to an analytical function for the percolation accessibility. They derived an equation to relate $\alpha(r)$ to the derivatives of the capillary pressure function P_c and percolation curves P_p . Then, they used a capillary tube model where $\alpha_{ca}(r) = \gamma \frac{dS_{nw}}{dP_c}$ (actually it should be $\alpha_{ca}(r) = \frac{dS_{nw}}{dP_c} \frac{P_c^2}{2\gamma}$) expressed in

terms of $\alpha(r)$ (input) and $\frac{dp}{dP_p}$ (function of the network size, N and the coordination number, z), i.e., $\alpha_{ca}(r) = \alpha(r) \frac{dP_p}{dp}$. Note that no P_c vs S_{nw} information enters in this equation from the left side and the result only reflects the accessibility function influence. They studied the influence of z and N . It was found that the larger the N and the smaller the z , the more skewed the distribution. They also proposed an algorithm to iterate for the real size distribution, but it failed to converge. In their study, z and N were given.

Zhou and Stenby^[218] conducted bond invasion percolation process in 3-D regular lattices with trapping to study this problem. In their work, the influence of z and N on residual saturation was considered. They derived a similar equation as before for the trapped situation. Although the trapping mechanism was included in their percolation model, its effect, and the influence of N and z on the estimation of $\alpha(r)$ were not discussed. Their result was closer to the their input data but still away from accurate.

Apparently, the size distribution problem has not been solved. Based on the observation that the slow drainage of mercury injection, either by pressure or rate control, produces the same pressure envelope, which is same as the standard *IP* pressure envelope, we apply the *IP* theory to the network modeling of the mercury porosimetry study and systematically study the factors which influence its interpretation. A new algorithm is proposed to estimate more accurate size distribution using percolation theory and the capillary pressure curve. The effects of dimension (2D or 3D), network size, coordination number, various percolation models and trapping are discussed.

7.2 Theory

We consider 2D, 3D site and mixed bond-site network models and used different lattices to investigate their effects. As in the mixed bond-site network model, we assume that the bond and site distributions are independent. This is the most popular (although perhaps not the most accurate) model employed by most researchers. Furthermore, often, only the bond size distribution is needed.

Assume that a size distribution function, $\alpha(r)$, is used to generate a pore network. Then a percolation process is conducted on this network. From percolation theory, the open fraction is $p = \int_{r_d}^{\infty} \alpha(r) dr$ and $\alpha(r) = -dp/dr_d$. Also, it is assumed that the capillary pressure is $P_c = 2\gamma/r_d$. The *nw* phase has the distribution

$$\alpha_{nw} = \begin{cases} \frac{\alpha(r)}{p} & r \geq r_d \\ 0 & r < r_d \end{cases}$$

Thus

$$S_{nw} = \frac{P_p \int_0^{\infty} \alpha_{nw}(r) v(r) dr}{\int_0^{\infty} \alpha(r) v(r) dr} \quad (141)$$

where P_p is the percolation probability. Now,

$$\frac{dS_{nw}}{dP_c} = -\frac{r_d^2}{2\gamma} \frac{dS_{nw}}{dr_d},$$

and

$$\frac{dS_{nw}}{dr_d} = -\left(\frac{P_p}{p}\right)' \alpha(r_d) \frac{\int_{r_d}^{\infty} \alpha(r) v(r) dr}{\int_0^{\infty} \alpha(r) v(r) dr} - \frac{P_p}{p} \frac{\alpha(r_d) v(r_d)}{\int_0^{\infty} \alpha(r) v(r) dr}$$

thus

$$\frac{dS_{nw}}{dP_c} = \frac{r_d^2}{2\gamma} \frac{\alpha(r_d)}{\int_0^{\infty} \alpha(r) v(r) dr} \left[\left(\frac{P_p}{p}\right)' \int_0^{\infty} \alpha(r) v(r) dr + \frac{P_p}{p} v(r_d) \right] \quad (142)$$

If we assume $v(r)$ constant, then

$$\frac{dS_{nw}}{dP_c} = \frac{r_d^2 \alpha(r_d)}{2\gamma} \left[\frac{P_p}{p} + p \left(\frac{P_p'}{p} - \frac{P_p}{p^2} \right) \right] = \frac{r_d^2 \alpha(r_d)}{2\gamma} \frac{dP_p}{dp} \quad (143)$$

Finally, we get

$$\alpha(r_d) = \frac{dS_{nw}}{dP_c} \frac{dp}{dP_p} \frac{2\gamma}{r_d^2} = \frac{dS_{nw}}{dP_c} \frac{dp}{dP_p} \frac{P_c^2}{2\gamma} \quad (144)$$

This is the basic equation for a site or bond percolation approach to estimate $\alpha(r)$.

For the capillary tube model, $p = P_p$ and we get the very simple result

$$\alpha(r) = \frac{dS_{nw}}{dP_c} \frac{P_c^2}{2\gamma} \quad (145)$$

For a mixed bond-site network model, the above theory is still applicable. P_p and S are functions obtained from the invasion site cluster fraction. The capillary pressure is $P_c \sim 1/r_b$, where r_b is the invading bond radius and p equals p_b , also calculated from the bond network, where the volume fraction of bonds is neglected. Finally, because $v(r)$ is constant, $S_{nw} = P_p$.

The typical steps of the algorithm in using equation (144) are as follows. For a given S , use the P_c curve to find P_c and $\frac{dS}{dP_c}$, then from the computed $p - P_p$ curve find $\frac{dp}{dP_p}$ and calculate $\alpha(r)$. In this approach, because two derivatives are used, the resulting $\alpha(r)$ is very noisy if only one realization is used for the construction of each curve.

In the derivation of the equation for $\alpha(r)$, we used $S_{nw} = P_p$ and $\alpha(r) = -\frac{dp}{dr}$. From this, we could directly use S to get $r = \frac{2\gamma}{P_c(S)}$ and to construct the $p(r)$ curve, from which the derivative of $\alpha(r)$ can be obtained. In this way, only one derivative is used. Further more, if we consider that $F(r_d) = \int_{r_{min}}^{r_d} \alpha(r) dr = 1 - \int_{r_d}^{\infty} \alpha(r) dr = 1 - p$, we can see that we actually *do not* need to use any derivatives at all for obtaining $F(r)$. In fact, the information content of $F(r)$ and $\alpha(r)$ is equivalent, while the noise is considerably reduced.

Using the above idea, we have a very simple, new algorithm to estimate the pore size distribution. For given z and N , the percolation curve, $P_p(p)$ can be constructed, where

multiple realization averages may be needed. For every S obtained from the $P_c(S)$ curve, $r(P_c(S))$ can be calculated and the corresponding $p(r)$ can be interpolated, say, by cubic spline interpolation. The $F(r) = 1 - p(r)$ so obtained is the estimated cumulative distribution function.

7.3 Simulations

Given a network geometry and structure (dimension, coordination number and known size distribution function), *Monte Carlo* simulations were performed to construct percolation and capillary pressure curves. We used various input size distribution functions to simulate the effect of the distribution function, which included Rayleigh, uniform and bi-Rayleigh functions. The Rayleigh distribution has the form

$$\alpha(r) = \frac{\pi}{2} \frac{(r - r_0)}{(r_a - r_0)^2} \exp\left[-\frac{\pi}{4} \frac{(r - r_0)^2}{(r_a - r_0)^2}\right]; \quad r_0 < r \quad (146)$$

where r_0 is the minimum size, r_a is the average size and its variance is $\sigma^2 = \frac{4-\pi}{\pi}(r_a - r_0)^2$. A uniform distribution is given by

$$\alpha(r) = \frac{1}{r_1 - r_0} \quad (147)$$

where r_0, r_1 are minimum and maximum sizes, respectively. It has a mean of $(r_0 + r_1)/2$ and a variance of $(r_1 - r_0)^2/12$. Finally, a bi-Rayleigh distribution function was also used,

$$\alpha(r) = \begin{cases} v_1 \frac{\pi}{2} \frac{r - r_{01}}{(r_{a1} - r_{01})^2} \exp\left[-\frac{\pi}{4} \frac{(r - r_{01})^2}{(r_{a1} - r_{01})^2}\right] & \text{if } r < r_{02} \\ v_1 \frac{\pi}{2} \frac{r - r_{01}}{(r_{a1} - r_{01})^2} \exp\left[-\frac{\pi}{4} \frac{(r - r_{01})^2}{(r_{a1} - r_{01})^2}\right] + v_2 \frac{\pi}{2} \frac{r - r_{02}}{(r_{a2} - r_{02})^2} \exp\left[-\frac{\pi}{4} \frac{(r - r_{02})^2}{(r_{a2} - r_{02})^2}\right] & \text{if } r \geq r_{02} \end{cases} \quad (148)$$

where $r_{01} < r_{02}$ and r_{01} is the minimum size and $v_1 + v_2 = 1$.

We used various percolation models, including ordinary site percolation (*OP*) in 2D (square and triangular lattice) and 3D (cubic lattice) and 3D invasion percolation (site and mixed bond-site, with and without trapping), to estimate the network size distribution $F(r)$ and compare it with the input (theory) function. The percolation curve was obtained by averaging multiple realizations or a single realization as specified, while the P_c curve was usually from one realization to mimic a practical situation.

The following procedure was followed in preparing the P_p and P_c curves. In all cases in the P_p calculation, we used a fixed uniform or Rayleigh distribution. In the *OP* simulations, r is increased from r_{min} to r_{max} . For each r , values of p and P_p or P_p and $P_c(r)$ are calculated, where P_p is the cluster fraction connected to entrance, and $P_c(r) = \frac{1}{r}$. In the site *IP* simulation, at each invasion step, we have $p = \int_{r_d}^{\infty} \alpha(r) dr$, $P_c = \frac{1}{r_d}$ and P_p is the fraction of the invaded cluster, where r_d is the minimum site radius in the invaded region. Data are not necessarily recorded at each invasion step.

In mixed bond-site IP , at each invasion step, the invaded sites are counted to calculate the saturation, S , and P_p (notice that in each step a new site is not necessarily added to the site cluster). The variables r , p and P_c are calculated from the invaded bond cluster. Here, r_d is the minimum bond size invaded. When we studied the effect of volume, the saturation was obtained by calculating each invaded site volume (assumed a ball for 3D, or a unit height disk for 2D) and added up all site volumes in the invaded area.

7.4 Results and Discussions

7.4.1 Size Distribution Interpreted by OP Simulation.

We first tested distribution functions interpreted by capillary pressure in OP , with the same network size for a pair of P_p and P_c data.

We conducted OP in 2D square lattice ($z = 4$), triangular lattice ($z = 6$) and 3D cubic ($z = 6$) lattices to see the geometry influence on the interpreted size distribution. A fixed network size and the same geometry were taken for both P_c and P_p data. The input Rayleigh distribution had $r_0 = 0$ and $r_a = 5$. Simulation results are shown in Figures 94 - 96 for 2D square, 2D triangular and 3D cubic lattices, respectively. The network sizes are specified in the figure captions. In Figure 94, the P_p curve is an average of 100 realizations. This is actually not necessary. From other experiments, we found that data averages of two-to-three sets are sufficient to get a smooth interpretation. Even one realization can still give acceptable results, except for the somewhat fluctuating character of the $F(r)$ curve. The P_c data were obtained from one realization. If we use more realizations, we actually get a perfect matching without any fluctuations whatsoever. In Figure 95, the P_p data are from an average of 10 realizations. Shown are three sets of P_c data with different random seeds, interpreted with the same P_p data. All of them show a close match with the theoretical curve. A similar situation is shown in Figure 96, where a nearly exact match is observed. By comparing the three cases, we can see that a 3D large lattice could offer us a real size distribution. Small network sizes do not lead to a perfect matching because of fewer data points. Also shown in these figures are the capillary tube model results. It is seen that more than half of the sizes are misinterpreted, all large sizes being interpreted as sizes corresponding to the middle point of the $F(r)$ curve. The derivative curve, $\alpha(r)$, in this case would involve a sharp spike, following which $\alpha(r)$ approaches 0. It can be concluded that the larger the sample size, the better the estimate and there is no influence of z on estimate of size distribution. This is in contrast to Mishra and Sharma^[217] as we discussed in introduction. Their results are really influenced by the possible mismatch in the z and N between the P_p and P_c networks.

Figure 94: Cumulative probability distribution curve $F(r)$ interpreted with ordinary percolation in 2D square site lattices of size 800x800. P_p from 100 realizations average, P_c from one realization. The solid line is the input distribution and the dotted lines are interpreted. The notation “cap. tube” is from the capillary tube model. The input Rayleigh distribution for P_c has parameters $r_0 = 0$ and $r_a = 5$.

Figure 95: Cumulative probability distribution curve $F(r)$ interpreted with ordinary percolation in 2D triangular site lattices of size 800x800. P_p from 10 realizations average, P_c from one realization. The solid line is the input distribution and the dot, dash-dot and dash lines are interpreted from three realizations. The notation “cap. tube” is from the capillary tube model. The input Rayleigh distribution for P_c has parameters $r_0 = 0$ and $r_a = 5$.

Figure 96: Cumulative probability distribution curve $F(r)$ interpreted with ordinary percolation in 3D cubic site lattices of size 80x80x80. P_p from 20 realizations average, P_c from one realization. The solid line is the input distribution and the dot, dash-dot and dash lines are interpreted from three realizations. The notation “cap. tube” is from the capillary tube model. The input Rayleigh distribution for P_c has parameters $r_0 = 0$ and $r_a = 5$.

7.4.2 Effect of Different Distributions on the Interpretation of the Capillary Pressure.

We tested distribution functions interpreted by capillary pressure from OP in various lattices with the same network size for a pair of P_p and P_c data, and with uniform and bi-Rayleigh input distributions.

Here, we tested the sensitivity to different input size distributions. The input uniform distribution had parameters $r_0 = 0$ and $r_1 = 15$, the bi-Rayleigh had parameters $r_{01} = 0$, $r_{a1} = 5$, $r_{02} = 10$, $r_{a2} = 15$, $v_1 = v_2 = 0.5$. Results are shown in Figure 97 - 99. Although a rather small size of 200x200 is used to interpret the data in Figures 97 and 98, the distribution features are quite well captured. With a 3D 80x80x80 cubic network the bi-Rayleigh distribution is exactly retrieved, where we actually used only one realization to get the P_p data.

We also tested IP on 2D and 3D site lattices. A typical IP example is shown in Figure 100. It was found that the same information as OP can be obtained.

7.4.3 Effect of a Mismatch of Network Sizes on the Interpretation of Capillary Pressure

Here, we used different network sizes to calculate the two different P_p and P_c curves. (See Figure 101 - 105). When P_p is generated from a larger size (N) network than for P_c , the obtained $F(r)$ underestimates the actual input curve, such that in the large pore size range,

Figure 97: Cumulative probability distribution curve $F(r)$ interpreted with ordinary percolation in 2D square site lattices of size 200x200. P_p from 100 realizations average, P_c from one realization. The solid line is the input distribution and the dot, dash-dot and dash lines are interpreted from three realizations. The notation “cap. tube” is from the capillary tube model. The input uniform distribution for P_c has parameters $r_0 = 0$ and $r_1 = 15$.

Figure 98: Cumulative probability distribution curve $F(r)$ interpreted with ordinary percolation in 2D square site lattices of size: a, 200x200; b, 800x800. P_p from 100 realizations average, P_c from one realization. The solid line is the input distribution and the dot, dash-dot and dash lines are interpreted from three realizations. The notation “cap. tube” is from the capillary tube model. The input bi-Rayleigh distribution for P_c has parameters $r_{01} = 0$ and $r_{a1} = 5$, $r_{02} = 10$, $r_{a2} = 15$, $v_1 = v_2 = 0.5$.

Figure 99: Cumulative probability distribution curve $F(r)$ interpreted with ordinary percolation in 3D cubic site lattices of size $80 \times 80 \times 80$. P_p from one realization, P_c from one realization. The solid line is the input distribution and the dot, dash-dot and dash lines are interpreted from three realizations. The notation “cap. tube” is from the capillary tube model. The input bi-Rayleigh distribution for P_c has parameters $r_{01} = 0$ and $r_{a1} = 5$, $r_{02} = 10$, $r_{a2} = 15$, $v_1 = v_2 = 0.5$.

Figure 100: Cumulative probability distribution curve $F(r)$ interpreted with invasion percolation in 3D cubic site lattices of size $60 \times 60 \times 60$. P_p from five realizations average, P_c from one realization. The solid line is the input distribution and the dot, dash-dot and dash lines are interpreted from three realizations. The notation “cap. tube” is from the capillary tube model. The input Rayleigh distribution for P_c has parameters $r_0 = 0$ and $r_a = 5$.

the smaller sizes are underestimated, while the larger ones are overestimated. The middle and small size parts are not influenced by the network size, however. The influence of this size effect is decreasing as both P_p and P_c network sizes increase (compare Figure 104 and Figure 105). This may imply that for practical core mercury injection, the size effect may be negligible because cores have large sizes. This, however, requires that the corresponding percolation curve should also be prepared on a sufficiently large network.

7.4.4 Effect of z on the Interpretation of Capillary Pressure

In practice, it may be difficult to know the true coordination number of the core. We considered the effect of different z in calculating P_p and P_c curves. We used triangular ($z = 6$) and square ($z = 4$) lattices to prepare P_p and P_c curves (see Figure 106). When a higher than the true z is used, the estimated $F(r)$ lies above the actual, i.e., large sizes are underestimated. Otherwise, the opposite is true. For a mixed bond-site percolation model, this influence will be discussed further.

7.4.5 Effect of Trapping on the Interpretation of Capillary Pressure

In slow drainage, many cases involve trapping. We would like to understand its effect on the interpretation of the distribution function. IP with trapping on a 3D site network was considered. The result is shown in Figure 107. The trapping effect appeared near the point where the invaded phase lost continuity (percolation threshold). Different realizations are observed to have a larger influence on the part where trapping occurred. Because the number of sites trapped depends on the realization, i.e., each run has a different residual saturation, we used only one realization of P_p to interpret the distribution curve (the end points vary among different realizations). Also, we noted that there is information lost for a small fraction of small pore sizes. These two effects may decrease at large network size.

7.4.6 Effect of Mixed Bond-Site Percolation

The most relevant model to a practical application is mixed bond-site invasion percolation. Typical IP curves, P_p vs p ($=p_b$, bond fraction), and the capillary pressure curve P_c vs S , are shown in Figure 111. We note that the percolation function P_p is different than before. When p approaches 1, P_p does not converge to a unique curve like the previous. This is quite important.

We considered a standard cubic mixed bond-site lattice to study the various factors discussed before. The estimated $F(r)$ curve is shown in Figure 108. We note that even with this more realistic model, the interpreted curve captures most of the original distribution. In fact, with a network size as large as $60 \times 60 \times 60$, the detectable part is nearly perfectly matching the true curve. However, even though no trapping exists (it was not considered here), information is lost for the fraction of small size bonds, because when all sites are

Figure 101: Cumulative probability distribution curve $F(r)$ interpreted with ordinary percolation in 2D square site lattices. P_p from 100 realizations average with lattice size of 200x200, P_c also from 100 realizations average. The solid line is the input distribution. The interpreted lines are from different P_c curves on lattice size of 50x50 (:-) (50 runs for average P_c), 100x100 (:), 200x200 (-.), 500x500 (-.-) and 800x800 (-) (from bottom to top), respectively. The notation “cap. tube” is from the capillary tube model. The input Rayleigh distribution for P_c has parameters $r_0 = 0$ and $r_a = 5$.

Figure 102: Cumulative probability distribution curve $F(r)$ interpreted with ordinary percolation in 2D square site lattices. P_p from 100 realizations average with lattice size of 200x200, P_c from one realization. The solid line is the input distribution. The interpreted lines are from different P_c curves on lattice size of 50x50 (:-), 100x100 (:), 200x200 (-.), 500x500 (-.-) and 800x800 (-) (from bottom to top), respectively. The notation “cap. tube” is from the capillary tube model. The input uniform distribution for P_c has parameters $r_0 = 0$ and $r_1 = 15$.

Figure 103: Cumulative probability distribution curve $F(r)$ interpreted with ordinary percolation in 2D square site lattices. P_p from 100 realizations average with lattice size of 200x200, P_c from one realization. The solid line is the input distribution. The interpreted lines are from different P_c curves on lattice size of 50x50 (:-), 100x100 (:), 200x200 (-.), 500x500 (-.-) and 800x800 (-) (from bottom to top), respectively. The notation “cap. tube” is from the capillary tube model. The input bi-Rayleigh distribution for P_c has parameters $r_{01} = 0$, $r_{a1} = 5$, $r_{02} = 10$, $r_{a2} = 15$, $v_1 = v_2 = 0.5$.

Figure 104: Cumulative probability distribution curve $F(r)$ interpreted with ordinary percolation in 3D cubic site lattice. P_p from 50 realizations average with lattice size $40 \times 40 \times 40$. The Solid line is the input distribution and the interpreted lines are from different P_c on lattice sizes of $20 \times 20 \times 20$ (100 realizations) (-.) and $80 \times 80 \times 80$ (20 realizations) (:). The notation “cap. tube” is from the capillary tube model. The input Rayleigh distribution for P_c has parameters $r_0 = 0$ and $r_a = 5$.

Figure 105: Cumulative probability distribution curve $F(r)$ interpreted with ordinary percolation in 3D cubic site lattice. P_p is from one realization with lattice size $120 \times 120 \times 120$. The Solid line is the input distribution and the interpreted lines are from different P_c on lattice sizes of $120 \times 120 \times 120$ (dot), $165 \times 165 \times 165$ (dash), and $90 \times 90 \times 90$ (dash-dot, two runs). The notation “cap. tube” is from the capillary tube model. The input Rayleigh distribution for P_c has parameters $r_0 = 0$ and $r_a = 5$.

Figure 106: Cumulative probability distribution curve $F(r)$ interpreted with ordinary percolation in 2D square and triangular site lattices with size 800x800. The Solid line is the input distribution and the interpreted lines are from P_c on square lattice (100 realizations average) and P_p on triangular lattice (10 realizations average) (dot) and from P_c (triangular lattice) and P_p (square lattice), the other way around (dash). The notation “cap. tube” is from the capillary tube model. The input Rayleigh distribution for P_c has parameters $r_0 = 0$ and $r_a = 5$.

Figure 107: Cumulative probability distribution curve $F(r)$ interpreted with invasion percolation in 3D cubic lattice with size 40x40x40. Both P_p and P_c are single realization (with different seed). The solid line is the input distribution and the interpreted line (dot) is from P_p by seed1 and P_c by seed2 and (dash) the other way around, i.e., P_p by seed2 and P_c by seed1. The notation “cap. tube” is from the capillary tube model. The input Rayleigh distribution for P_c has parameters $r_0 = 0$ and $r_a = 5$.

Figure 108: Cumulative probability distribution curve $F(r)$ interpreted with invasion percolation in 3D mixed bond-site lattices of size $60 \times 60 \times 60$. The P_p curve is an average of 3 realizations, the P_c curves correspond to one realization. The solid line is the input distribution and the interpreted dot, dash-dot and dash lines are from three P_c realizations. The notation “cap. tube” is interpreted from the capillary tube model. The input Rayleigh distribution for P_c has parameters $r_0 = 0$ and $r_a = 50$.

invaded, there still remain many small bonds not yet invaded, and their further invasion, although it raises P_c , does not give any new information on S (the bonds do not contain volume). We note that the missing fraction does not decrease when the network size increases, thus it is practically independent of size. The capillary tube model for this problem gives a much worse interpretation. In addition to missing the fraction of small sizes, which is the same for both models, middle sizes are underestimated, and large sizes are severely overestimated. The effect of different N used in the P_p and P_c curves, has a similar result as before, i.e., if N is overestimated (larger than the value of P_c network), the $F(r)$ curve is underestimated (under the true curve), otherwise, it is overestimated (above the true curve) (see Figure 109). We expect that the size effect will be small or disappear when the network size is large and/or both sizes are as close as possible. When trapping is considered, a quite large part (small and middle size) of the bond size distribution information is lost (see Figure 110). If a process involves trapping, we predict that no useful information on the size distribution information could be obtained. Fortunately, in mercury injection, there is a negligible trapping effect.

7.4.7 Effect of Mixed Bond-Site Invasion with Randomized Coordination Number z .

From the previous effect of z in 2D, we expect that a larger effect would be exerted in this case. In fact, even in the absence of trapping, the effect of different z in P_p and P_c curves

Figure 109: Cumulative probability distribution curve $F(r)$ interpreted with invasion percolation in 3D mixed bond-site lattices. P_p curve is an average of 5 realizations with lattice size of $40 \times 40 \times 40$ and P_c curves correspond to 3 realizations. The solid line is the input distribution, the different interpreted lines are from different P_c on lattice sizes of $60 \times 60 \times 60$ (dot), $40 \times 40 \times 40$ (dash) and $30 \times 30 \times 30$ (dash-dot). The notation “cap. tube” is interpreted from the capillary tube model. The input Rayleigh distribution for P_c has parameters $r_0 = 0$ and $r_a = 50$.

Figure 110: Cumulative probability distribution curve $F(r)$ interpreted with invasion percolation in 3D mixed bond-site lattices of size $40 \times 40 \times 40$. Trapping effect is considered. P_p curve is an average of 3 realizations (taking shortest data length) and P_c curves correspond to one realization. The solid line is the input distribution, the interpreted dot, dash-dot and dash lines are from three P_c realizations. The notation “cap. tube” is interpreted from the capillary tube model. The input Rayleigh distribution for P_c has parameters $r_0 = 0$ and $r_a = 50$.

Figure 111: *IP* on 3D mixed bond-site lattice of size 40x40x40: (a) Accessibility function P_p , for different z equal to 3, 4, 5, 6 from left to right, (b) Capillary pressure curve P_c , for different z equal to 3, 4, 5, 6 from top to bottom.

is large. We used a randomized z to simulate a 3D lattice with average $z \neq 6$. Similar to [204], when assigning bond sizes drawn from a given distribution function, we used another independent uniformly distributed [0,1] random number to decide whether the bond should be blocked, with a probability $1 - z/6$. If the independent random number was less than this probability, the bond radius was assigned to zero. Otherwise, the drawn size was assigned as the bond size.

Using the same network size and z for both P_p and P_c , we conducted simulations for z varying between 3 to 6. The corresponding accessibility functions P_p and the P_c curves are shown in Figure 111. The interpreted distribution functions are shown in Figure 112 - 114 for $z=3, 4, 5$, respectively. (For $z = 6$, refer to Figure 108). All cases show the correct estimate of the real distribution function. It is interesting to note that when z is small, such as $z = 3$, nearly the whole distribution function is interpreted, with a negligible missing fraction at small sizes. This is understandable, because when z is small, a site is connected to fewer sites and a higher percentage of bonds is needed to invade all sites at the end of *IP*. (Certainly in the limit of a single bond-site tube model ($z = 2$), all bonds must be invaded in order to invade all sites.)

We next considered the effect of mismatch of z on the interpretation of the data. The results are shown in Figure 115 - 117. Figure 115 shows a case in which z has a large effect. Unlike the previous situation (Figure 106), where only the middle portion of the distribution function is distorted, here, the whole distribution curve is shifted above and to the right of the real distribution, if P_p has a z larger than in P_c , and shifted to the left and under the real distribution, if P_p has a z smaller than in P_c .

Figure 112: Cumulative probability distribution curve $F(r)$ interpreted with invasion percolation in 3D mixed bond-site lattices of size $40 \times 40 \times 40$, average $z = 3$. The P_p curve is an average of 3 realizations and the P_c curves correspond to one realization. The solid line is the input distribution and the interpreted dot, dash-dot and dash lines are from three P_c realizations. The notation “cap. tube” is interpreted from the capillary tube model. The input Rayleigh distribution for P_c has parameters $r_0 = 0$ and $r_a = 50$.

Figure 113: Cumulative probability distribution curve $F(r)$ interpreted with invasion percolation in 3D mixed bond-site lattices of size $40 \times 40 \times 40$, average $z = 4$. The P_p curve is an average of 3 realizations and the P_c curves correspond to one realization. The solid line is the input distribution and the interpreted dot, dash-dot and dash lines are from three P_c realizations. The notation “cap. tube” is interpreted from the capillary tube model. The input Rayleigh distribution for P_c has parameters $r_0 = 0$ and $r_a = 50$.

Figure 114: Cumulative probability distribution curve $F(r)$ interpreted with invasion percolation in 3D mixed bond-site lattices of size $40 \times 40 \times 40$, average $z = 5$. The P_p curve is an average of 3 realizations and the P_c curves correspond to one realization. The solid line is the input distribution and the interpreted dot, dash-dot and dash lines are from three P_c realizations. The notation “cap. tube” is interpreted from the capillary tube model. The input Rayleigh distribution for P_c has parameters $r_0 = 0$ and $r_a = 50$.

7.4.8 Effect of Mixed Bond-Site Network Model, with Real Volume Saturation.

The final effect we would like to address is the effect of volume. All the previous simulations were based on the number fraction to get the saturation for the P_c curve, namely we used the approximation of constant volume for all sites. In reality, however, we only measure the volume saturation for the capillary pressure curve, not the number fraction of invaded sites. Here, we tested the validity of this approximation. In order to calculate the volume saturation, we distributed site sizes according to a Rayleigh distribution with $r_0 = 50$ and $r_a = 200$. This broad distribution gives sufficient variation of saturation values. As we expect, the volume saturation does not result in significant differences with the curve obtained based on the site number fraction. Figure 118 shows an example of a network of size $40 \times 40 \times 40$. Similar results were obtained for a $20 \times 20 \times 20$ network. In a real system, the network size may be much larger than in these tests and we expect that results based on the number fraction of invaded sites to be as good as the volume saturation, thus percolation theory could be applied using the accessibility function.

7.4.9 Another Way of Interpreting Mercury Capillary Pressure Curves.

In 1980, Wall and Brown^[214] were among the first to apply percolation theory in adsorption-desorption processes. In their work, they used ordinary percolation and focused on the largest percolation cluster. They found that P_p is a unique function of the product of coordination number with the bond open fraction (only showed data in the neighborhood

Figure 115: Cumulative probability distribution curve $F(r)$ interpreted with invasion percolation in 3D mixed bond-site lattices of size $40 \times 40 \times 40$. The P_p is an average of 3 realizations for any given z and the P_c corresponds to one realization. The solid line is the input distribution. The three lines (dot, dash-dot, dash) above the real curve are interpreted from three runs of P_c with $z = 3$ against the average P_p with $z = 6$. The three lines (dot, dash-dot and dash) below the real curve are interpreted from three runs of P_c with $z = 6$ against the average P_p with $z = 3$. The notation "cap. tube" is from the capillary tube model. The input Rayleigh distribution for P_c has parameters $r_0 = 0$ and $r_a = 50$.

Figure 116: Cumulative probability distribution curve $F(r)$ interpreted with invasion percolation in 3D mixed bond-site lattices of size $40 \times 40 \times 40$. The P_p is an average of 3 realizations for any given z and the P_c corresponds to one realization. The solid line is the input distribution. The three lines (dot, dash-dot and dash) above the real curve are interpreted from three runs of P_c with $z = 4$ against the average P_p with $z = 6$. The three lines (dot, dash-dot and dash) below the real curve are interpreted from three runs of P_c with $z = 6$ against the average P_p with $z = 4$. The notation "cap. tube" is from the capillary tube model. The input Rayleigh distribution for P_c has parameters $r_0 = 0$ and $r_a = 50$.

Figure 117: Cumulative probability distribution curve $F(r)$ interpreted with invasion percolation in 3D mixed bond-site lattices of size $40 \times 40 \times 40$. The P_p is an average of 3 realizations for any given z and the P_c corresponds to one realization. The solid line is the input distribution. The three lines (dot, dash-dot and dash) above the real curve are interpreted from three runs of P_c with $z = 5$ against the average P_p with $z = 6$. The three lines (dot, dash-dot and dash) below the real curve are interpreted from three runs of P_c with $z = 6$ against the average P_p with $z = 5$. The notation "cap. tube" is from capillary the tube model. The input Rayleigh distribution for P_c has parameters $r_0 = 0$ and $r_a = 50$.

Figure 118: Cumulative probability distribution curve $F(r)$ interpreted with invasion percolation in 3D mixed bond-site lattices of size $40 \times 40 \times 40$. The P_p curve is an average of 5 realizations and the P_c curves correspond to one realization. The solid line is the input distribution, dot lines are interpreted from P_c curves with volume saturation, dash lines are interpreted from P_c curves with number fraction. a, b and c are three realizations of P_c . d shows an example of P_p and S vs p plot. The input Rayleigh distribution for P_c has parameters $r_0 = 0$ and $r_a = 50$.

of percolation point in their paper). This result has its origin on the theory of finite-size effects in percolation. They tested FCC (face centered cubic), BCC (body faced cubic), cubic and tetrahedral lattices, and found the approximate result $zp_c \approx 1.4$ which is very close the conjecture $zp_c \approx \frac{d}{d-1} = 1.5$ ^{[219][220]}. We extend this idea to the entire range of the percolation accessibility function. (Figure 119). It is found that with the exception of a slight deviation at high value of P_p for $z = 3$, we obtained an almost unique curve, from our available randomized z range. This information could be very useful in interpreting the mercury curve. Namely, we could obtain the P_p vs zp curve by assuming a coordination number and performing the percolation simulation. By interpreting the mercury porosimetry data from the P_p vs zp curve, we obtain a zp vs r curve, and further, the $F(r) = 1 - p$ vs r curve, given the correct z information. Following this procedure, we obtained P_p vs zp data for four networks with $z = 6, 5, 4$ and 3 , and interpreted the corresponding P_c against these data sets. The results are shown in Figures 120 - 122. In these figures, the solid lines are the zp curve calculated from networks with the same z as P_c . Other lines are interpreted. We can see that for $zp \leq 2$, all interpreted curves match pretty well with the corresponding theoretical curves. At the percolation point ($zp_c \approx 1.5$) an "exact" match is noticed. From these figures, one could draw a horizontal line from the point $zp = 1.5$, the intercept of which with each curve gives r_c , the percolation radius, hence the percolation saturation from the P_c curve, which may be useful for calculating z .

Now, if we assume that we have information on z for each interpreted curve, we can divide the zp value by z to get p or $F(r) = 1 - p$ vs r , which is the desired information.

7.5 Conclusions

In part, we studied various effects in the estimation of the pore size distribution from mercury pressure data with percolation theory. We first proposed a new algorithm to interpret mercury porosimetry data to obtain the pore size distribution. The most practical and useful network model, namely the mixed bond-site network model, suffers from some mismatch of the effect of z . For given z with a sufficiently large network, of size as close as possible to the real, the proposed new algorithm can estimate a much more accurate pore size distribution than other currently available methods. Experimental data are needed to confirm the above algorithm. We also found that when we use a size similar to or as large as the core sample size, the effect of mismatch in size is negligible.

We also discussed the physical limitation of the mercury injection capillary pressure curve to obtain small size distribution information if a porous medium has a large coordination number. In particular, if trapping occurs, the resulting capillary pressure curve cannot reliably be analyzed for the size distribution. Fortunately, mercury porosimetry is not subject to trapping. Also, it was found that the volume distribution of size does not affect the results obtained. This is very useful, as it allows the direct use of percolation accessibility curves.

Figure 119: Accessibility function P_p vs zp for IP in 3D mixed bond-site lattice with size $40 \times 40 \times 40$. The solid, dot, dash-dot and dash denote $z = 3, 4, 5$ and 6 , respectively.

Figure 120: zp distribution interpreted from the capillary pressure curve using IP in 3D mixed bond-site lattices with size of $40 \times 40 \times 40$. The P_p vs zp curve is from a $z = 6$ lattice (three runs average). The P_c curves are obtained from different z lattices (one run). The solid lines are calculated from a network with the z value being the same as that of corresponding P_c 's. The other lines are interpreted with different z for P_c , namely $z = 3$ (:-), 4 (- -), 5 (-.) and 6 (:). The corresponding capillary tube $p \sim r$ predictions are also shown. The input Rayleigh distribution for P_c has parameters $r_0 = 0$ and $r_a = 5$.

Figure 121: zp distribution interpreted from the capillary pressure curve using IP in 3D mixed bond-site lattices with size of $40 \times 40 \times 40$. The P_p vs zp curve is from a $z = 5$ lattice (three runs average). The P_c curves are obtained from different z lattices (one run). The solid lines are calculated from a network with the z value being the same as that of corresponding P_c 's. The other lines are interpreted with different z for P_c , namely $z = 3$ (:-), 4 (- -), 5 (-.) and 6 (:). The corresponding capillary tube $p \sim r$ predictions are also shown. The input Rayleigh distribution for P_c has parameters $r_0 = 0$ and $r_a = 5$.

Figure 122: zp distribution interpreted from the capillary pressure curve using IP in 3D mixed bond-site lattices with size of $40 \times 40 \times 40$. The P_p vs zp curve is from a $z = 3$ lattice (three runs average). The P_c curves are obtained from different z lattices (one run). The solid lines are calculated from a network with the z value being the same as that of corresponding P_c 's. The other lines are interpreted with different z for P_c , namely $z = 3$ (:-), 4 (- -), 5 (-.) and 6 (:). The corresponding capillary tube $p \sim r$ predictions are also shown. The input Rayleigh distribution for P_c has parameters $r_0 = 0$ and $r_a = 5$.

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