XVIII International Conference on Water Resources
CMWR 2010
J. Carrera (Ed)
CIMNE, Barcelona 2010

A MULTI-SCALE APPROACH TO MODEL TWO-PHASE FLOW IN HETEROGENEOUS POROUS MEDIA

Christos D. Tsakiroglou

Foundation for Research and Technology Hellas - Institute of Chemical Engineering and High Temperature Chemical Processes (FORTH/ICE-HT)
Stadiou street, Platani, 26504 Patras, Greece
e-mail: ctsakir@iceht.forth.gr, web page: http://www.iceht.forth.gr

Key words: Multi-scale models, two-phase flow, heterogeneous media, relative permeability, capillary pressure, network analysis

Summary. *The immiscible displacement of a wetting fluid by a non-wetting one in heterogeneous porous media is modeled by using a multi-scale network-type analysis: (1) The pressure-controlled immiscible displacement of water by oil in pore-and-throat networks (length scale~1mm) is controlled by capillary forces. (2) The pressure-controlled immiscible displacement in uncorrelated or spatially correlated cubic lattices (length scale~1cm) is governed by capillary and gravity forces. At this scale, each node represents a network of the previous scale. (3) The rate-controlled immiscible displacement of water by oil in cubic networks (length scale~10cm), where each node represents a lattice of the previous scale, is simulated by accounting for capillary, gravity and viscous forces. The multi-scale approach along with the pore structure properties of soils can be employed to determine the transient responses of the pressure drop and axial distribution of water saturation, and estimate the effective (up-scaled) relative permeability functions, at the soil column scale.*

1 INTRODUCTION

The general procedure for the determination of the effective two-phase flow coefficents (relative permeability functions, capillary pressure curve) of soils is based on the interpretation of two-phase flow tests on soil columns with the aid of inverse modeling algorithms[1,2]. Microscopic pore structure analysis[3] along with immiscible and miscible displacement experiments performed on undisturbed soil columns[4,5] revealed that the microporous matrix of mineral soils, composed of sand, clay and silt, is strongly heterogeneous, and the flow pattern is dominated by preferential flowpaths. Under such conditions the applicability of the conventional macroscopic equations of the two-phase flow equations becomes questionable[5]. However, there is a lack of robust approaches that will enable us to examine the effects of multi-scale heterogeneities on the transient flow pattern and effective two-phase flow coefficients.

The effects of pore structure statistics and topology on the effective two-phase flow coefficients can be examined by using mechanistic quasi-static[6] or dynamic[7,8] pore network simulators of the immiscible displacement of two fluids. When simulating the contaminant transport in a reservoir, the macroscopic two-phase flow equations are solved at scales (0.1-

1m) which are much larger than that of a pore network (~0.001-0.01m). Given that the viscous and gravity terms become pronounced at the scale of the numerical grid, computational tools are required to incorporate the soil heterogeneities up to the grid scale into the relative permeability curves (up-scaling)[9,10].

In the present work, we develop a computational procedure that allows the calculation of the effective relative permeability curves of a heterogeneous soil column by employing as input data the statistics of pore space properties (length scale~1mm), and the permeability distribution at the scale of a cluster of pore networks (length scale~1cm) and the scale of a network of such clusters (length scale~10cm). A pore network model, a large-scale site percolation model, and a dynamic large-scale network simulator are employed successively in order to produce the capillary pressure and relative permeability curves at the three-scales, by using as input parameters for each scale the results of the previous one.

2 PORE NETWORK MODEL

The broad pore and throat radius distributions produced by the precise characterization of the pore space of mineral soils[3] are decomposed into several narrow component distribution functions. These component distribution functions are employed for the computer-aided construction of Euclidean pore-and-throat networks. The pore space is modeled as a three-dimensional network of "spherical" pores interconnected through "circular" and volumeless throats (primary porosity). The pore-diameter distribution (PSD), throat-diameter distribution (TSD), and primary porosity, ε_p, are used as input parameters for the construction of the primary network. The fractal porosity is regarded as roughness features along the pore-walls and is quantified by the ratio of secondary to total porosity, $A = \varepsilon_f / \varepsilon_t$, and fractal dimension D_s. For the calculation of hydraulic conductivity the concept of the constricted unit cell of sinusoidal shape is adopted[3].

2.1 Calculation of capillary pressure and relative permeability curves

The quasi-static oil/water drainage in a network is simulated by tracking the motion of menisci according to the capillary resistance encountered in throats and calculating the fluid saturation at each value of the capillary pressure when equilibrium is established. The hydraulic conductivity and the subsequent 1st scale relative permeability of each phase are calculated by imposing a pressure difference across it, "freezing" the other phase, formulating mass balances at each node (pore centre), solving the system of linear equations, and determining the pressure field. Two opposite sides of the network serve as entrance and exit, whereas periodicity is imposed along the other boundaries. The simulated capillary pressure curves of several realizations (with the network permeability k spanning some orders of magnitude) are fitted with the following models

$$P_{co} = c\gamma_{ow} \cos\theta \, k^{-\delta} \tag{1}$$

$$\left(S_w - S_{wi}\right)/\left(1 - S_{wi}\right) = \left(P_c / P_{co}\right)^{-1/m} - h_c \tag{2}$$

where P_c is the capillary pressure, P_{co} is the entry pressure, γ_{ow} is the oil/water interfacial tension, θ is the contact angle, S_w is the water saturation, S_{wi} is the irreducible water saturation, and c,δ,m,h_c are parameters to estimate. Respectively, the simulated water and oil relative permeabity curves are fitted with the following models

$$k_{rw} = a_w\left(\frac{S_w - S_{wi}}{1 - S_{wi}}\right)^{e_{w1}} + \left(1 - a_w\right)\left(\frac{S_w - S_{wi}}{1 - S_{wi}}\right)^{e_{w2}} \tag{3}$$

$$k_{ro} = k_{ro}^0\left[a_o\left(\frac{1 - S_w}{1 - S_{wi}}\right)^{e_{o1}} + \left(1 - a_o\right)\left(\frac{1 - S_w}{1 - S_{wi}}\right)^{e_{o2}}\right] \tag{4}$$

where $a_w, e_{w1}, e_{w2}, k_{ro}^0, a_o, e_{o1}, e_{o2}$ are parameters to estimate.

3 LARGE-SCALE SITE PERCOLATION MODEL

A cluster of pore networks can be regarded as a cubic lattice of nodes each representing a pore network with its flow properties $[k, P_c\left(S_w; k\right), k_{rw}\left(S_w\right), k_{ro}\left(S_w\right)]$ obtained from pore network simulations. The very broad range of pore length scales probed in soils[3] is reflected in a broad distribution $f_1\left(k^*; \sigma_{k1^*}\right)$ of the dimensionless node (pore network) permeability ($k^* = k/\langle k \rangle$) where σ_{k1^*} is the standard deviation. Depending on whether the permeabilities are assigned randomly or non-randomly to the nodes, an uncorrelated or spatially correlated permeability field may arise. The computer-aided construction of a spatially correlated cubic lattice of nodes is based on the approach reported in Tsakiroglou and Payatakes[11]. The overall permeability of the network is calculated by imposing a pressure difference across it, determining the influx rate with numerical solution of mass balances at nodes, and fitting the results to Darcy law.

The quasistatic downward flow of oil in an initially water-occupied network is simulated as a site percolation process[12]. For a current value of the external pressure P_e, the network is scanned to identify the nodes that have access to oil phase and satisfy the condition

$$P_e \geq P_{co} + \left(\rho_w - \rho_o\right)gh \tag{5}$$

where ρ_w, ρ_o are the water and oil density, respectively, and h is the vertical distance of a node from the top. Oil invades these nodes and water saturation is calculated according to Eq.(2) by setting

$$P_c = P_e - \left(\rho_w - \rho_o\right)gh \tag{6}$$

Eq.(2) is also used to update the fluid saturation in each node occupied by both fluids. The procedure is iterated until no change of water saturation occurs. Afterwards, the external

pressure is increased by a finite step and the calculations are repeated. The relative permeability functions resulting from pore network analysis are regarded identical for all nodes and used to compute the hydraulic conductance of each phase. The 2nd scale water and oil relative permeability curves are determined by imposing a pressure drop across the lattice and adopting a procedure similar to that followed in pore network approach. The simulation stops when no more changes of water saturation are observed any more. Finally, the simulated results are fitted with Eqs.(1)-(4) to estimate new parameter values of fitting functions

4 DYNAMIC LARGE-SCALE NETWORK SIMULATOR

Permeabilities are assigned to the nodes of the large network according to the permeability distribution function $f_2\left(k^*;\sigma_{k2^*}\right)$. The results of site percolation model along with Eqs.(1)-(4) are used to express the capillary pressure of each node as a function of local permeability and water saturation and the water & oil relative permeability of each node as function of water saturation. The gravity is incorporated into the local capillary pressure by defining the piezometric capillary pressure

$$P_c'\left(k,S_w\right)=P_c\left(k,S_w\right)+\left(\rho_w-\rho_o\right)gh \tag{7}$$

For each node j, the effective oil, $g_{o,j}$, and water, $g_{w,j}$, conductance are calculated in accordance to the relationships

$$g_{o,j}=l_N k_j k_{ro}\left(S_{w,j}\right)/\left(\kappa\mu_w\right) \qquad g_{w,j}=l_N k_j k_{rw}\left(S_{w,j}\right)/\mu_w \tag{8}$$

where μ_w,μ_o are the water and oil viscosities, l_N is the node length, and $\kappa=\mu_o/\mu_w$ is the viscosity ratio. When both fluids coexist in a node, its total conductance is obtained with volume averaging, according to the relation

$$g_j=1\Big/\left(\frac{h_{w,j}}{g_{w,j}}+\frac{h_{o,j}}{g_{o,j}}\right) \tag{9}$$

by using the water and oil weight fractions

$$h_{w,j}=\frac{S_{w,j}}{1-S_{wi}}-\frac{S_{wi}}{1-S_{wi}} \qquad h_{o,j}=1-h_{w,j} \tag{10}$$

In order to calculate the flow rate between adjacent nodes, we define unit cells, each consisting of the 1/6th of two adjacent nodes. The volumetric flow rate through each unit cell, q_{ij}, is given by

$$q_{ij}=g_{ij}\left(P_i-P_j-\Delta P_{c,ij}\right) \tag{11}$$

where the conductance of the cell g_{ij} is given by

$$g_{ij}=2g_i g_j/\left(g_i+g_j\right) \tag{12}$$

P_i, P_j are the pressures at the centres of adjacent nodes, and $\Delta P_{c,ij}$ is an additional pressure drop due to the capillary pressure. Assuming that the algebraic sum of the volumetric flow rates of unit cells adjoining to each node is equal to zero (mass balance), we get a system of coupled linear equations the solution of which provides the instantaneous pressure field of the network. The current flow rates of the invading fluid in each unit cell are utilized to calculate the time spans required for its partial filling (5-10%) with oil. The calculation of the time spans is restricted to unit cells where both fluids coexist. Afterwards, the minimum time span Δt_{min} is determined. Assuming pseudo steady-state conditions, the water and oil saturation in each unit cell (and hence in each node) at the end of the time interval, Δt_{min}, are updated according to the instantaneous flow rate, namely

$$\left(V_{w,ij}\right)_{t+\Delta t_{min}} = \left(V_{w,ij}\right)_t - \Delta t_{min} q_{ij} \tag{13}$$

In order to calculate the up-scaled oil and water relative permeability functions, a constant pressure difference is imposed across the network, mass balances are applied to each node, and the system of coupled linear equations is solved. The overall oil and water outflow rates along with the pressure difference are finally introduced into the integrated form of the two-phase flow Darcy equations.

The pressure difference across the large-scale network is so adjusted that the overall oil influx rate Q_{net} is kept close to the target flow rate Q_{oil}. The overall influx flow rate Q_{net} of the injected fluid (oil) is calculated for several (4-5) values of the pressure difference, ΔP_{net}, imposed across the network, by solving the system of coupled linear equations obtained with mass balances at nodes. The results are fitted to the linear relationship:

$$\Delta P_{net} = A Q_{net} + B \tag{14}$$

so that the parameters A, B are estimated. Afterwards, Eq.(14) is employed to compute ΔP_{oil} for the target flow rate Q_{oil}. Then, setting $\Delta P_{net} = \Delta P_{oil}$, network analysis is reused to examine whether the calculated total flow rate $Q_{o,net}$ deviates from its target value Q_{oil}. If the deviation exceeds 1%, then the pressure difference in next iteration $i+1$ is updated according to

$$\Delta P_{net,i+1} = \Delta P_{net,i} - A\left(Q_{net,i} - Q_{oil}\right) \tag{15}$$

and the calculations are repeated until convergence is attained. The procedure is repeated until oil breakthrough to occur and both the total oil saturation and total pressure drop across the network do not change any more.

5 RESULTS AND DISCUSSION

The methodology was applied to the datasets of an undisturbed and heterogeneous soil column that was used extensively in earlier multiphase transport studies[4,5]. The parameter values of the fluid system n-dodecane / NaCl aqueous solution ($\gamma_{ow} = 50$mN/m , $\theta = 6^o$) were used. Two-phase flow in pore networks was simulated for 5 realizations by sampling the component pore and throat size distributions from the complete ones of sample C7[3]. Although

the 1st scale simulated $k_{rw}(S_w), k_{ro}(S_w)$ and S_{wi} are sensitive to pore size statistics and subsequently to absolute permeability (Fig.1a,b), for the sake of simplicity, in the next scale of simulation, the relative permeability functions of nodes were represented by identical fitting functions whereas the S_{wi} value was kept constant (Table 1).

Parameter	1st scale simulations	2nd scale simulations	Parameter	1st scale simulations	2nd scale simulations
c	7.29	5.51	a_w	0.161	1.0
δ	0.3494	0.351	e_{w1}	0.855	3.52
S_{wi}	0.633	0.678	e_{w2}	4.247	-
m	0.107	0.406	a_o	1.0	0.129
h_c	$8.1\text{x}10^{-7}$	$1.6\text{x}10^{-11}$	e_{o1}	1.738	1.836
			e_{o2}	-	1.820

Table 1: Estimated parameter values of fitting functions

In order to simulate a cluster of networks with a very broad range of permeabilities[3], a log-normal distribution with $\sigma_{k1^*} = 2$ was used as input parameter and spatially correlated permeability fields of varying average permeability were built. The 2nd scale simulated $k_{rw}(S_w), k_{ro}(S_w), P_c(k; S_w)$ curves along with the fitting functions (Table 1) are shown in Fig.2.

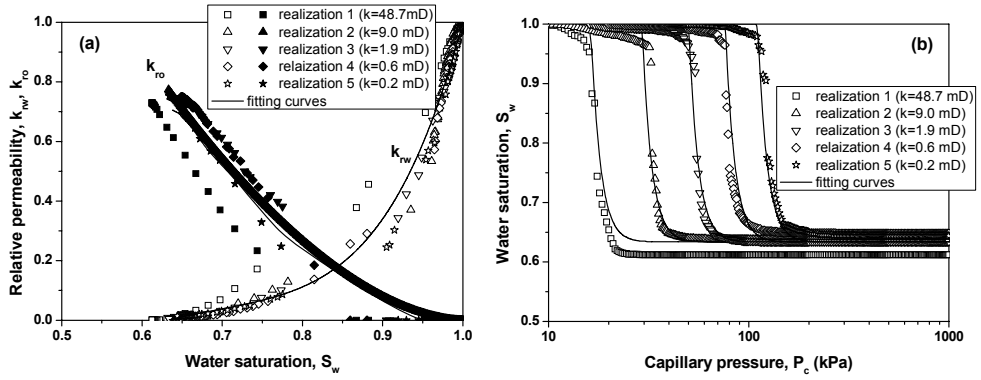

Figure 1: (a) Relative permeability and (b) capillary pressure curves from pore network simulations (1st scale two-phase effective flow coefficients)

The rate-controlled ($Ca = 5x10^{-8}$) immiscible displacement was simulated in uncorrelated and correlated large-scale networks, differing with respect to σ_{k2^*} (=0.2,0.5,0.8) of the input log-normal permeability distribution function. The 3rd scale (up-scaled) water and oil relative permeability functions have the tendency to increase and decrease, respectively, with the width of permeability distribution increasing, whereas the spatial correlations have a weak effect on them (Fig.3a,b). The simulated transient responses of the pressure drop across the network and the axial distribution of water saturation (Fig.4a,b) are comparable to corresponding experimental results[5]

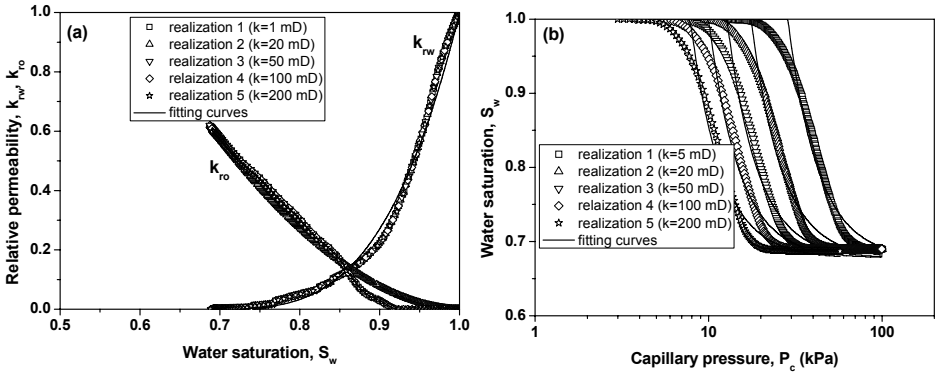

Figure 2: (a) Relative permeability and (b) capillary pressure curves from large-scale site percolation model (2nd scale two-phase effective flow coefficients)

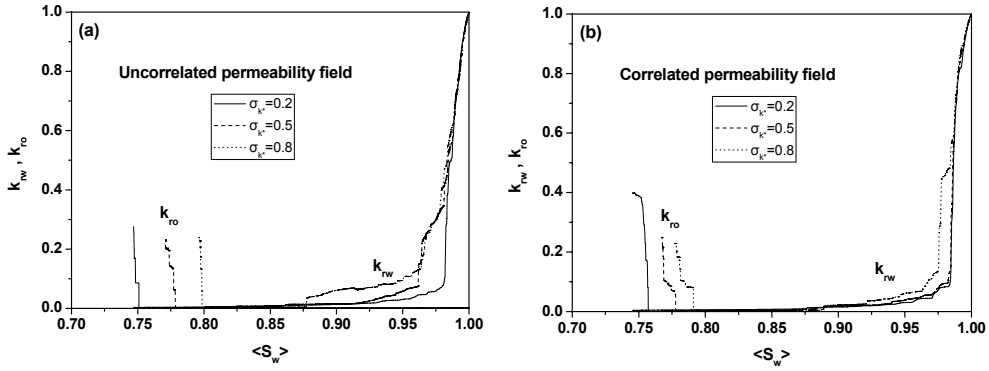

Figure 3: Relative permeability curves from dynamic large-scale network simulator for (a) uncorrelated and (b) correlated permeability field (3rd scale two-phase effective flow coefficients)

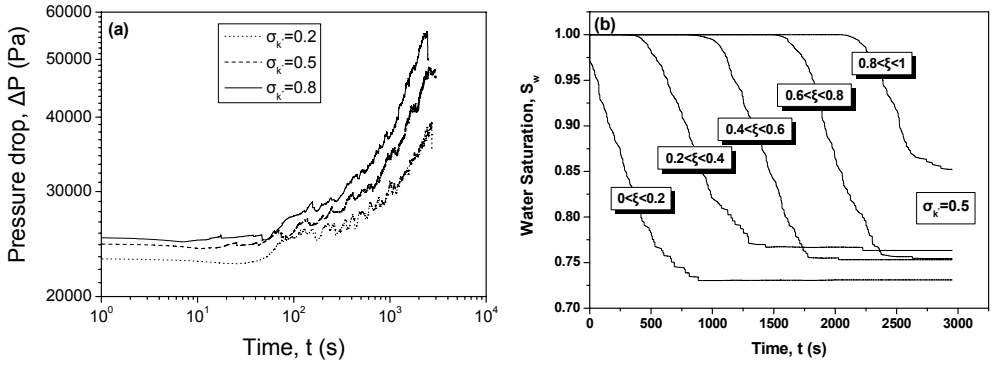

Figure 4: Simulated transient responses of the (a) pressure drop and (b) axial distribution of water saturation at the soil column scale

6 CONCLUSIONS

A methodology is suggested to compute the up-scaled relative permeability functions of

heterogeneous soil columns from micro-structural information. The oil/water immiscible displacement is simulated at three successive scales each dominated by different flow mechanisms: (1) the pore network approach is governed by capillarity; (2) the large-scale site percolation model is dominated by capillary and gravity forces; (3) the large-scale rate-controlled displacement is governed by the interaction of capillary, gravity and viscous forces. The effective two-phase flow coefficients calculated at each scale of simulation are fed as input data to the next scale. The methodology is demonstrated with its application to the prediction of the properties of an undisturbed soil column[5].

REFERENCES

[1] M. Inoue, J. Simunek, S. Shiozawa and J.W. Hopmans, "Simultaneous estimation of soil hydraulic and solute transport parameters from transient infiltration experiments", *Adv. Water Resour.*, **23**, 677-688 (2000).

[2] C.A. Aggelopoulos and C.D. Tsakiroglou, "The effect of micro-heterogeneity and capillary number on capillary pressure and relative permeability curves of soils" *Geoderma*, **148**, 25-34 (2008).

[3] C.D. Tsakiroglou and M.A. Ioannidis, "Dual-porosity modeling of the pore structure and transport properties of a contaminated soil", *Eur. J. Soil Sci.*, **59**, 744-761 (2008).

[4] C.A. Aggelopoulos and C.D. Tsakiroglou, "Quantifying soil heterogeneity from solute dispersion experiments", *Geoderma*, **146**, 412-424 (2008).

[5] C.A. Aggelopoulos and C.D. Tsakiroglou, "A multi-flow path approach to model immiscible displacement in undisturbed heterogeneous soil columns", *J. Contam. Hydrol.*, **105**, 146-160 (2009).

[6] C. Laroche and O. Vizika, "Two-phase flow properties prediction from small-scale data using pore network modeling", *Transp. Poorus Media*, **61**, 77-91 (2005).

[7] M. Singh and K.K. Mohanty, "Dynamic modeling of drainage through three-dimensional porous materials", *Chem. Eng. Sci.*, **58**, 1-18 (2003).

[8] B. Markicevic, A. Bazylad and N. Djilali, "Determination of transport parameters for multiphase flow in porous gas diffusion electrodes using a capillary network model", *J. Power Sources*, **171**, 706-717 (2007).

[9] L.M. Abriola and G.F. Pinder, "A multiphase approach to the modeling of porous media contamination by organic compounds. 2. Numerical simulation", *Water Resour. Res.*, **21**, 19-26 (1985).

[10] B.H. Kueper and E.O. Frind, "Two-phase flow in heterogeneous porous media. 2. Model application", *Water Resour. Res.*, **27**, 1059-1070 (1991).

[11] C.D. Tsakiroglou and A.C. Payatakes, "Effects of pore-size correlations on mercury porosimetry curves", *J. Colloid Interface Sci.*, **146**, 479-494 (1991).

[12] M.A. Ioannidis, I. Chatzis and F.A.L. Dullien, "Macroscopic percolation model of immiscible displacement: effects of buoyancy and spatial structure", *Water Resources Research***, 23**, 3297-3310 (1996).