To the Graduate Council:

I am submitting herewith a dissertation written by Abdullah Cihan entitled “Flow and Transport in Unsaturated Porous Media: Fractal Modeling, Analytical Solutions and Experimentation.” I have examined the final electronic copy of this dissertation for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Doctor of Philosophy, with a major in Biosystems Engineering.

John S. Tyner, Major Professor

We have read this dissertation and recommend its acceptance:

Ed Perfect

Jaehoon Lee

Randall W. Gentry

Accepted for the Council:

Carolyn R. Hodges
Vice Provost and Dean of the Graduate School

(Original signatures are on file with official student records)
FLOW AND TRANSPORT IN UNSATURATED POROUS MEDIA: FRACTAL MODELING, ANALYTICAL SOLUTIONS AND EXPERIMENTATION

A Dissertation
Presented for the
Doctor of Philosophy Degree
The University of Tennessee, Knoxville

Abdullah Cihan
May 2008
DEDICATION

This dissertation is dedicated to my parents, Asuman Cihan and Kemal Cihan, and my wife, Sidika Pinar Turkbey Cihan.
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ABSTRACT

This dissertation consists of five parts, each describing a specific topic of unsaturated flow and transport. The first three parts describe the development of soil hydraulic function models with the effects of partial drainage by using fractal and probabilistic approaches. During drainage of a porous medium, both the pore size distribution and the connectivity of pores determine the drained pore volume as function of suction. New analytical expressions were presented for the water retention (part 1), intrinsic permeability (part 2), and relative permeability (part 3) functions. Predictions based on the analytical models are compared with estimates of the intrinsic permeability \( k \) derived from lattice Boltzmann method (LBM) simulations of saturated flow in virtual representations of classical (deterministic) and randomized Menger Sponges. Overall, the analytically predicted \( k \) values matched the \( k \) values from the LBM simulations with less than 14% error for deterministic sponges with minimum pore sizes ranging from \( 1/3^1 \) to \( 1/3^4 \). We presented a new approach that allows the prediction of relative permeability by direct use of measured water retention data without fitting. This new discrete model describes the drained pore space and permeability at different suctions incorporating the effect of both pore size distribution and connectivity among water-filled pores. We tested the performance of the new model by comparing its predictions of relative permeability to those of van Genuchten-Mualem (VG-M). Overall, the new method (RMSE=0.175, LRMSE=1.101) predicted the measured relative permeability data better than the VG-M model (RMSE=0.216, LRMSE=2.381). Part 4 presents analytical solutions of the advective solute transport in a macropore with simultaneous diffusion into an unbounded
soil matrix. We obtained three sets of exact and approximate solutions for various boundary and initial conditions. Part 5 presents a moisture moment method to estimate unsaturated soil hydraulic properties. By analyzing the change in forces of two load cells that suspend either end of a soil column and the inlet water pressure, the unsaturated hydraulic conductivity and water retention functions are obtained. We applied the method to a sandy silt loam and the analyses show the method is promising.
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PART I
WATER RETENTION MODELS FOR SCALE-VARIANT AND
SCALE-INVARIANT DRAINAGE OF MASS PREFRACTAL
POROUS MEDIA
Abstract

This research describes the development of water retention models incorporating the effects of partial drainage in random mass prefractal porous media. The pore-size distribution as well as the connectivity of pores determines the drained pore volume as a function of suction. The concept of probability of drainage leads to a general scale-variant model (GM) in which the proportion of pores that drain at a given suction level is dependent on the fractal dimension of the drained pore phase, $D_d$, and the proportion of pores that drain at the first suction level or air entry value. Two simplified cases of the general model are also presented. The first simplified model (SC1) is a special case of the GM in which all of the largest pores drain completely at the first suction level. The second model (SC2) is a scale-invariant model in which the proportion of drained pores for each suction level remains constant and is obtained by setting $D_d$ equal to the mass fractal dimension, $D$, of the porous medium. Fitting each model to numerically simulated drainage curves for random 2-dimensional prefractal porous media with known $D$ values showed that the GM fitted the numerical data much better than either the SC1 or SC2 models, which were less flexible at high $D$ values. Estimates of $D_d$ for the GM and SC1 models approached $D$ when $D$ was less than the critical value for percolation, i.e. $D_c \sim 1.716$. Independent estimates of the probability of drainage indicate that the connectivity of water-filled pores decreases as a result of the lower porosities associated with higher $D$ values. A novel experimental protocol is suggested for testing these theoretical observations.
1. Introduction

The use of fractal methods for quantification of soil hydraulic functions is a powerful tool to understand the flow of fluids and contaminants in the unsaturated zone. Fractal models are based on physical parameters that lead to much easier interpretation compared to empirical models. Fractals are iterative geometrical models for describing irregular and fragmented systems. As such, they are ideally-suited to simulate the hierarchical and heterogeneous nature of soil structure.

Models based on fractal geometry are increasingly being used to derive physically-based expressions for soil hydraulic properties, particularly the saturation-capillary pressure curve (Giménez et al., 1997; Bird et al., 2000; Wang et al., 2005). One of the earliest and most widely accepted fractal water retention models was derived by Rieu and Sposito (1991). This model does not take into account the randomness of natural porous media and incomplete connectivity of individual pores which might result in partial drainage of pores. Numerical capillary drainage simulations in random fractal structures showed that a lack of pore connectivity in the Rieu and Sposito (1991) model caused deviations between predicted and observed data (Perrier et al., 1995; Bird and Dexter, 1997).

Perrier et al. (1999) proposed a pore-solid fractal model in which the initiator includes pores and solids, which have constant fractions, as well as an iterative phase space. The iterative phase vanishes as the iteration process approaches infinity. Bird et al. (2000) presented a water retention function based on the pore-solid fractal approach. Wang et al. (2005) tested Bird et al.’s (2000) model against a very large data set for different types of soils by fitting the model to experimental data. Their results indicate
that Bird et al.’s (2000) function provides a better fit than the Rieu and Sposito (1991) and Brooks and Corey (1964) equations, which are shown to be simplified cases of the pore-solid fractal model.

Fractal water retention equations, including Bird et al.’s (2000) model, are often used to estimate the fractal dimension of the porous medium. During drainage of a fractal porous medium, both the fractal dimension and the connectivity of pores determine the drained pore volume as function of suction. However, since the above mentioned models do not incorporate the effect of pore connectivity explicitly, estimates of the fractal dimension obtained by fitting these models to experimental data may not be accurate. Rather they should be thought of as apparent fractal dimensions.

Perfect (2005) presented a water retention curve model introducing the concept of scale-invariant probability of drainage to account for incomplete pore drainage during monotonic drying of a random prefractal porous medium. The probability of drainage, \( P_d \), defined as the probability of pores of length \( l \) emptying during drainage, was stated to be scale-invariant. Although the final saturation-capillary pressure equation given by Eq. (15) in Perfect (2005) turns out to be correct, the derivation given in Perfect (2005) leads to a scale-variant probability in which the ratio of the number of drained pores to number of total pores changes at each iteration level of drainage. Thus, the conclusions drawn about the scale-invariant \( P_d \) parameter are not correct, and scale-invariant pore drainage can only be obtained as a simplified case of a more general model, which will be provided below.

The purpose of this article is to correct the error in the previous study by Perfect (2005) and to further explore modeling of partial drainage in a random mass prefractal
porous medium. We present soil water retention models for various cases of interest based on scale-variant and scale-invariant conceptualizations of incomplete pore drainage. The different assumptions involved are tested by fitting each model to the numerically simulated monotonic drainage curves for the random 2-dimensional prefractal porous media investigated by Sukop et al. (2001). Probabilities of drainage are also estimated from the drainage curves for comparison with the model assumptions.

2. Theory

Simplified soil water retention models for scale-variant and scale-invariant pore drainage will be derived as special cases of a more general model which is presented first.

2.1. General Fractal Drainage Model (GM)

The numbers of solids, $N_s$, and pores, $N_p$, of length $l$ in a mass prefractal porous medium are given by:

$$N_s(l) = l^{-D} = \left(b^i\right)^D$$

$$N_p(l) = n_p b^{(i-1)D} = \left(b^E - b^D\right)b^{(i-1)D}$$

where $i$ is the iteration level, $E$ is the Euclidean dimension, $D$ is the mass fractal dimension defined as $\log\left[N_s(l)/N_s(bl)\right]/\log b$, $b$ is the scale factor, and $n_p$ is the number of pores in the generator. As drying occurs, not all pores of a given size drain at the appropriate suction due to incomplete pore connectivity. The number of drained pores, $N_d$, is assumed to be fractal, and proportional to a power of the length $l$ as expressed by:

$$N_d(l) = P\left(b^E - b^D\right)b^{(i-1)D_i}$$
where $P$ is the ratio of the drained pore space to the total pore space in the generator, $0 \leq P \leq 1$, and $D_d$ is the fractal dimension for the drained pore space, which can be defined as:

$$D_d = \frac{\log \left[ \frac{N_d(l)}{N_d(b l)} \right]}{\log b} \leq D \quad (4)$$

The cumulative volume of the drained pore space, $V_d(l)$, can be calculated from Eq. (3) using the following expression:

$$V_d(l) = \sum_{n=1}^{i} \frac{N_d(l)}{b^{E_n}} = P \left( \frac{b^E - b^{D_d}}{b^E - b^{D_d}} \right) \left[ 1 - \left( \frac{1}{b^i} \right)^{E - D_d} \right] \quad (5)$$

where $\sum$ is the summation symbol and $1 \leq n \leq i$ is the $n^{th}$ iteration level. Then, the volumetric water content of the partially drained prefractal porous medium is given by:

$$\theta = \phi - V_d(l) = \phi - P \left( \frac{b^E - b^{D_d}}{b^E - b^{D_d}} \right) \left[ 1 - \left( \frac{1}{b^i} \right)^{E - D_d} \right] \quad (6)$$

Expressed in terms of relative saturation, $S$, Eq. (6) becomes:

$$S = 1 - \frac{P}{\phi} \left( \frac{b^E - b^{D_d}}{b^E - b^{D_d}} \right) \left[ 1 - \left( \frac{1}{b^i} \right)^{E - D_d} \right] \quad (7)$$

Invoking the Young-Laplace expression (de Gennes et al., 2004), $1/b^i$ in Eq. (7) can be replaced with the normalized capillary pressure, $h_{min}/h$, giving,

$$S = 1 - \frac{P}{\phi} \left( \frac{b^E - b^{D_d}}{b^E - b^{D_d}} \right) \left[ 1 - \left( \frac{h}{h_{min}} \right)^{D_d - E} \right] \quad (8)$$

which is identical to Eq. (15) in Perfect (2005). Eq. (8) reduces to the Rieu and Sposito (R&S) (1991) model when $P = 1$ and $D_d = D$.

An example realization of drainage for the general model (GM) with $P = 0.5$ and $D_d = 1.630\ldots$ in a random Sierpinski carpet of unit length constructed using $E = 2$, $b = 3$, 

---

6
$i = 2$, and $D = 1.771\ldots$ is presented in Figure 1.1(a). All tables and figures are located in the appendix. Since $P = 0.5$, only one of the largest pores of size of $1/b$ drains. At the second iteration level, $i = 2$, there are $N_p(1/b^2)$ pores and the proportion of those pores that drain is given by $P b^{D_d-D}$, i.e. six out of fourteen pores of size $1/b^2$ become empty (Figure 1.1a). (Figures and tables appear in the appendices.)

The sensitivity of Eq. (8) to the parameters $P$ and $D_d$ is demonstrated for a 3-dimensional mass prefractal porous medium or Menger sponge in Figure 1.2. Figure 1.2(a) shows changes in $S$ as function of $\log_b(h/h_{\min})$ while $P$ is varied from 0.1 to 1 and $D_d$ is kept constant at 2.5 ($< D = 2.680\ldots$). When $P$ is equal to unity, all the largest pores drain. The slope of the saturation versus normalized capillary pressure curve decreases as $P$ increases. Likewise, Figure 1.2(b) shows that $S$ decreases as $D_d$ increases from 2 to $D$. $S$ is most sensitive to $D_d$ at values approaching $D$, and $D_d$ has little impact on $S$ near the wet end of the water retention curve.

**Simplified Case 1 (SC1): Scale-variant**

If the probability of drainage in the generator, $P$, is assumed to be unity such that all the largest pores drain completely, Eq. (3) becomes

$$N_d(l) = (b^E - b^D) b^{(i-1)D_d}$$

and the relative saturation is now given by:

$$S = 1 - \frac{1}{\phi \left( b^E - b^{D_d} \right)} \left[ 1 - \left( \frac{h}{h_{\min}} \right)^{D_d-E} \right]$$

(10)
Figure 1.1(b) presents an example of drainage for the simplified scale-variant model (SC1) with $D_d = 1.630$. Since $P = 1$, both of the largest pores drain at first iteration level, while at the second iteration level, a $b^{D_d-D}$ fraction of the $N_p(1/b^2)$ pores drains, i.e. twelve out of fourteen pores sized $1/b^2$ become empty (Figure 1.1b).

**Simplified Case 2 (SC2): Scale-invariant**

When $D_d = D$, the ratio of the number of drained pores to total pores at any iteration level $i$ remains constant and equal to $P$. In this case, Eq. (3) is written as:

$$N_d(i) = P(b^E - b^D)b^{(i-1)D}$$

yielding the following relative saturation function:

$$S = 1 - \frac{P}{\phi} \left[ 1 - \left( \frac{h}{h_{\min}} \right)^{D-E} \right]$$

This equation has the same form as the water retention model for a pore-solid fractal proposed by Bird et al. (2000), although the interpretation of the model parameters is different.

Figure 1.1(c) presents an example of drainage for the scale-invariant model (SC2) with $P = 0.5$. At each iteration level, the ratio of the empty pores to filled pores is constant, i.e. at the first iteration level, one of the two pores of size $1/b$ drains, while at $i = 2$, seven out of the fourteen pores of size $1/b^2$ drain (Figure 1.1c).

**2.2. Probability of Drainage**

Perfect (2005) defined the probability of drainage at any level $n$ in the fractal hierarchy as the ratio of the number of drained pores to the total number of pores of length $l$, which was expressed as:
It was then assumed that the same proportions of pores empty at each iteration level, i.e. $P_d(l) = P_d(bl)$. However, this approach does not account for the continued drainage of pores of length $l$ at subsequent suction levels, or any imbibition of drainage water from previously non-drained pores of length $\geq bl$. In reality, the relationship between $P_d(l)$ and $P_d(bl)$ is much more complicated, and the cumulative effect of all inputs and outputs of water must be taken into account for each pore size class.

To further investigate the pore-scale drainage processes underlying the different analytical models in section 2.1 we present a new probabilistic expression for $N_d$ that incorporates the effect of connectivity among pores with different sizes and allows continuing drainage of pores of sizes $1/b^{i+1}$, $1/b^{i+2}$ etc. into pores of size $1/b^i$ at different suctions. A more appropriate form of the probability of drainage will also be formulated.

Depending upon the geometrical arrangement (lacunarity) of the prefractal porous medium, any pores of length $1/b$ that do not drain at the appropriate suction may remain full, or empty into pores of length $1/b^2$, $1/b^3$… or $1/b^i$ as $h \to \infty$. Similarly, non-draining pores of length $1/b$ may never empty, or later drain into pores of length $1/b^2$, $1/b^3$… or $1/b^i$ (Perfect, 2005). Drainage of the remaining water-filled pores from the first iteration level may continue at subsequent iteration levels.

At iteration level 1, which corresponds to the air entry value or minimum suction, a $P_1$ fraction times the volume of pores generated at $i = 1$ drains, i.e. $P_1 N_p^{(1)}/b^E$. At iteration level 2, a $P_2$ fraction of the pore volume generated at $i = 2$ plus the remaining pore volume from iteration level 1 drains, i.e. $P_2 [N_p^{(2)}/b^{2E} + (1-P_1) N_p^{(1)}/b^E]$. Then, after

\[
N_d(l) = \frac{N_d(l)}{N_p(l)} \tag{13}
\]
two iterations, the total volume of water remaining in pores of sizes $1/b$ and $1/b^2$ can be calculated as

$$
(1-P_2) \left[ \frac{N_p^{(2)}}{b^{2E}} + \left(1-P_1\right) \frac{N_p^{(1)}}{b^{E}} \right] = (1-P_2) \frac{N_p^{(2)}}{b^{2E}} + \left(1-P_2\right)\left(1-P_1\right) \frac{N_p^{(1)}}{b^{E}} \tag{14}
$$

At iteration level 3, the drained pore volume is the summation of $P_3$ times the volume of pores generated at $i=3$ and the remaining pore volume from iteration level 2. This conceptual model for the drainage process can be formulated as:

$$
n = 1 \quad \phi - \theta_1 = P_1 \frac{N_p^{(1)}}{b^{E}}
$$

$$
n = 2 \quad \theta_2 - \theta_1 = P_2 \left[ \frac{N_p^{(2)}}{b^{2E}} + \left(1-P_1\right) \frac{N_p^{(1)}}{b^{E}} \right]
$$

$$
n = 3 \quad \theta_3 - \theta_2 = P_3 \left[ \frac{N_p^{(3)}}{b^{3E}} + \left(1-P_2\right) \frac{N_p^{(2)}}{b^{2E}} + \left(1-P_2\right)\left(1-P_1\right) \frac{N_p^{(1)}}{b^{E}} \right]
$$

$$
\vdots\quad \vdots\quad \vdots
$$

$$
n = i \quad \theta_i - \theta_{i-1} = P_i \left[ \frac{N_p^{(i)}}{b^{iE}} + \left(1-P_{i-1}\right) \frac{N_p^{(i-1)}}{b^{(i-1)E}} + \cdots + \left(1-P_{i-1}\right)\left(1-P_{i-2}\right)\cdots\left(1-P_1\right) \frac{N_p^{(1)}}{b^{E}} \right]
$$

where $\theta_1, \theta_2, \theta_3, \ldots$ are the volumetric water contents corresponding to the suction levels $n = 1,2,3\ldots$ The probability of drainage of the remaining pore volume at any $i$ or any corresponding suction, $P_i$, can now be expressed as:

$$
P_i = \frac{\theta_i - \theta_{i-1}}{\sum_{n=1}^{i-1} \frac{N_p^{(n)}}{b^{nE}} \prod_{k=n}^{i-1} \left(1-P_k\right)} \tag{16}
$$

where $\prod$ is the product symbol and if $(i-1) < k$, $\prod_{k}^{i-1} \left(1-P_k\right) = 1$. In order to compare this approach with Eq. (3), the drained pore volume at iteration number $i$ can be expressed in
terms of $N_d$ and $b^i$ such that $\theta_{i-1} - \theta_i = N_d^{(i)} (1/b^i)$. Then, by rearranging Eq. (16), $N_d^{(i)} (l = 1/b^i)$ can be written as:

$$N_d^{(i)} = P_i b^{E_i} \sum_{n=1}^{i} \frac{N_p^{(n)}}{b^{E_n}} \prod_{k=n}^{i-1} (1-P_k)$$ (17)

The $P_i$ values in Eqs. (16) and (17) contain information about the connectivity of the pore system, and are independent of any assumed fractal drainage behavior. Each $P_i$ value is the percentage of the volume of the connected pores filled with water whose sizes are greater than or equal to $1/b^i$. At the appropriate suction level, $i$, those pores that are connected to the atmosphere will drain. If $b$, $D$, and $i$ values are known a priori for a fractal porous medium, then the $P_1$, $P_2$, ..., $P_i$ values can be estimated inversely from the resulting water retention curve. By inversely solving Eq (16) against drained pore volume data from the drainage simulations of Sukop et al. (2001) we can tell how $P_i$ changes as a function of iteration level and $D$. We can also test the implied assumption of power-law scaling in Eq. (3) by comparison with Eq. (17).

2.3. Methods

Simulated Water Retention Data

Bird and Dexter (1997) and Sukop et al. (2001) computed moisture suction relations in two-dimensional prefractal pore networks using an invasion percolation algorithm. They simulated drainage in $b = 3$ and $i = 5$ randomized Sierpinski carpets with different $D$ values by allowing three sides of each prefractal structure to be open to the atmosphere, while the bottom was connected to a water sink. According to their algorithm, at a given tension level $i$ all pores of size greater than $1/b^i$ that are filled with water and are connected to the atmosphere by at least one path consisting of pores no
smaller than $1/b^i$ drain. The simulations neglect the effect of pore coalescence and assume applicability of the Young-Laplace equation. Ten simulations were run for each set of carpet parameters.

**Non-linear Fitting**

Equations (8), (10) and (12) were fitted to the simulated water retention curves using non-linear regression (Marquardt method) in SAS (SAS Institute, 1999). Both $P$ and $D_d$ were estimated for the GM, while only $D_d$ was estimated for SC1 and $P$ for SC2. All of the fits converged according to the SAS default convergence criterion (SAS Institute, 1999). The balance between goodness-of-fit and parsimony for the different model fits was evaluated using Akaike’s information criterion (AIC). The AIC was estimated by (SAS, 1999):

$$
AIC = \nu \ln \left( \frac{ESS}{\nu} \right) + 2p
$$

where $\nu$ is the number of observations, ESS is the error sum of squares, and $p$ is the number of model parameters. The smaller (the more negative) the AIC value, the better the model.

**Inverse estimation of $P_i$**

By using the data obtained from the numerical simulations, the $P_i$'s in Eq. (16) can be calculated by explicitly solving Eq. (15) from the known values of water content versus iteration level since $b$, $D$ and saturated water content or porosity are known a priori. For example, at iteration level 1, $P_1 = (\phi - \theta_i)/(1 - b^{E-P})$. As an example of this
procedure, Table 1.2 shows the calculation of the $P_i$ values for water retention data from realization #1 of a $b = 3$, $i = 5$, $D = 1.771\ldots$ carpet. Since $N_p$ is known for these structures, $N_d$ can also be calculated from the resulting estimates of $P_i$.

3. Results and Discussion

The model equations represented by Eqs. (8), (10) and (12) were fitted to numerically simulated monotonic drainage curves for 10 realizations of each of three different generators ($b = 3$ and $D = 1.892\ldots$, $D = 1.771\ldots$ and $D = 1.630\ldots$) of random two-dimensional prefractal porous media (Sukop et al., 2001; Perfect, 2005). Since $D$, $b$ and $h_{min}$ were known from the simulations, these parameters were specified in the fitting procedure. The GM is represented by Eq. (8) with two unknown parameters: $P$ and $D_d$. The SC1 is represented by Eq. (10) with one unknown parameter: $D_d$. The SC2 is represented by Eq. (12) with one unknown parameter: $P$.

Figure 1.3 shows the differences in the performance of the three cases for each $D$ value investigated. The examples presented in Figure 1.3 were chosen from the realizations which gave the maximum difference in ESS values between the GM and SC1 and between the GM and SC2, respectively. Figure 1.3(a) presents the comparison of the GM and SC1 for the realization resulting in the maximum ESS difference when $D = 1.630\ldots$. The GM and SC1 result in similar predictions, and their ESS values are very close to each other. Likewise, in Figure 1.3b, the GM and SC2 almost overlap giving the same ESS values up to 4 digits. Figures 1.3(a) and 1.3(b) show that all of the models gave similar predictions to the numerical data for $D = 1.630\ldots$. However, for larger $D$ values (Figures 1.3c-f), the simplified scale-variant (SC1) and scale-invariant (SC2) models showed marked deviations, while the GM always fit the numerical data the best. The
R&S (1991) model always showed a large deviation from the simulations for all $D$ values investigated.

A summary of the different fits is presented in Table 1.1. Estimates of $D_d$ from the GM were greater than those from the SC1, and the maximum difference between the estimates of $D_d$ occurred at the highest $D$ value. Both sets of $D_d$ values approached $D$ when $D$ was less than the critical value for percolation, i.e. $D_c \sim 1.716…$ (Perfect, 2005). This suggests that a larger proportion of the pores drain due to higher pore connectivity when $D < D_c$. When $D > D_c$, the $D_d$ estimates were always smaller than $D$. The mean $P$ values increased with increasing $D_d$ and decreasing $D$. This trend was more pronounced for the SC2 than the GM, which produced estimates of $P$ much closer to unity.

Overall, the mean ESS for the nonlinear fits ranged from 0.001 and 0.048. As can be seen from Table 1, the GM has the lowest ESS values for all of the $D$ values and also the lowest Akaike information criterion (AIC) values for the two largest $D$ values. All of the cases were very similar for the lowest $D$ value investigated. These results indicate that the GM represented by Eq. (8) is the best fitting model overall. For systems well below the percolation threshold, the SC2 is a viable alternative since it fits just as well as the GM, but has one less parameter.

The probabilistic expression developed for the drained pore volume, Eq. (16), was inversely solved for $P_i$ and $N_d$ using the same simulated water retention curves from Sukop et al. (2001). Figure 1.4 shows how the mean $P_i$ values calculated from ten realizations for each $D$ value change as function of suction level. The mean $P_i$ for each $D$ investigated generally decreases with suction level except for $D = 1.630…$ which shows a less pronounced trend, fluctuating between 0.63 and 0.86. Decreasing $P_i$ values with
increasing $D$ indicate that the connectivity of water-filled pores decreases as a result of the lower porosity of the randomized two-dimensional carpets with higher mass fractal dimensions. The error bars show one standard deviation around the mean and their high values indicate a high degree of variability among the ten different realizations.

Predicted relationships for $N_d$ using the mean parameter estimates from Table 1.1 in Eq. (3) compared favorably with the inversely calculated $N_d$ values from Eq. (17) (Figure 1.5). This result confirms a power law-type behavior for the drained pore space, and the applicability of Eq. (3), at least for random mass prefractal porous media that drain according to the simple invasion percolation algorithm of Bird and Dexter (1997). Further research will be required to evaluate these equations against drainage data simulated using alternative techniques (e.g., lattice Boltzmann) and/or measured on natural porous media. In this context, pore-scale observations of the partitioning of air and water within pores at a given suction level would be particularly useful. An epoxy casting technique developed by Wunderlich (1985) could be used for this purpose. In this technique, air is forced into a soil sample initially saturated with a colored epoxy representing water. After equilibration at a given suction, the epoxy is solidified in situ. Finally, thin sections of the sample are prepared to image the phase distributions.

We have shown in section 2.1 that the assumption $D_d = D$ leads to a theoretical water retention curve, Eq. (12), that is of the same form as the drainage model for a pore-solid fractal proposed by Bird et al. (2000). However, $P$ in the present model represents the scale-invariant probability of drainage, while in Bird et al. (2000) this parameter controls the void: solid ratio at each iteration level, and ultimately the porosity. Thus, while Eq. (15) in Perfect (2005) is correct, it is for general scale-variant drainage rather
than scale-invariant drainage. Furthermore, Eq. (7) in Perfect (2005) is incorrect and there is no simple way of relating $D_d$ to $D$ unless $D << D_c$. This means that estimates of $D_d$ from saturation-capillary pressure data cannot be used to infer values of the underlying mass fractal dimension of the porous medium unless it is assumed that scale-invariant drainage has occurred or that $D << D_c$. Pore-scale experiments and percolation studies are needed to assess the extent to which these assumptions apply to natural porous media.

By fitting different drainage models to the numerical simulations of Sukop et al. (2001) it was possible to identify the model that best fits saturation-capillary pressure data when $D$, $b$ and $h_{min}$ are known (i.e. the GM). This would not have been possible with experimentally determined water retention curves since these parameters are not known a priori for natural porous media. For soil data sets, Eqs. (8), (10) and (12) all take on the same form, which can be written for the purpose of fitting as:

$$S = 1 - \frac{\alpha}{\phi} \left[ 1 - \left( \frac{h}{h_{min}} \right)^{\beta - E} \right]$$

(19)

where $\alpha$ and $\beta$ represent the different compound parameters for each case. Perfect (2005) already showed that Eq. (19) provides an excellent fit to water retention curves for six Washington State soils investigated by Campbell and Shiozawa (1992). Based on the present study, we still interpret the estimates of $\alpha$ and $\beta$ obtained by fitting Eq. (19) to these data as $P(b^E - b^D)/(b^E - b^{D_d})$ and $D_d$, respectively. However, it is no longer possible to relate these parameters to the mass fractal dimensions of the different soils.
4. Conclusions

Theoretical water retention equations for a prefractal porous medium have been presented for three cases based on scale-variant and scale-invariant conceptualizations of incomplete pore drainage. The scale-variant drainage models, GM and SC1, allow the proportion of non-draining pores, \( P_d \), to change with pore size and suction level, while in the scale-invariant model, SC2, \( P_d \) is a constant. Overall, best estimates of the simulated data were obtained for the GM. For systems well below the percolation threshold, however, the SC2 (which is equivalent to a pore-solid fractal model) is preferred since it fits just as well as the GM and has one less unknown parameter.

We have presented a new probabilistic expression for the drained pore space that incorporates the effect of connectivity among pores with different sizes and allows continuing drainage of pores at different suctions. Extracting an analytical expression for the water content based on this new approach is currently not possible without knowing \( P_i \) or \( 1-P_i \), or assuming a specific type of distribution as a function of suction level. However, the conceptualization seems promising for future work towards developing a more complete physical model that explicitly includes the effects of both connectivity and fractal dimension. Further work is also required to extend the approaches presented in this study to scale-variant and scale-invariant wetting processes in order to derive expressions for the main wetting branch and scanning loops of the water retention curve. Experimental studies of partial drainage and wetting at the pore-scale would also be valuable for model validation purposes.
LIST OF REFERENCES
References


APPENDIX
Table 1.1. Mean values of the parameter estimates and goodness-of-fit statistics (ESS = error sum of squares and AIC = Akaike information criterion) for the different models fitted to the simulated water retention curves from Sukop et al. (2001) using nonlinear regression. Standard deviations are given in the parenthesis.

<table>
<thead>
<tr>
<th>Model</th>
<th>Type</th>
<th>$D$</th>
<th>$D_d$</th>
<th>$P$</th>
<th>ESS</th>
<th>AIC</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>1.630…</td>
<td>1.630 (0.002)</td>
<td>0.923 (0.017)</td>
<td>0.016 (0.019)</td>
<td>-35.2 (7.5)</td>
</tr>
<tr>
<td>GM</td>
<td>1.771…</td>
<td>1.521 (0.247)</td>
<td>0.819 (0.135)</td>
<td>0.011 (0.017)</td>
<td>-39.8 (8.8)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.892…</td>
<td>1.279 (0.367)</td>
<td>0.807 (0.377)</td>
<td>0.001 (0.001)</td>
<td>-55.0 (6.8)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.630…</td>
<td>1.568 (0.015)</td>
<td>-</td>
<td>0.024 (0.025)</td>
<td>-34.4 (7.0)</td>
<td></td>
</tr>
<tr>
<td>SC1</td>
<td>1.771…</td>
<td>1.292 (0.186)</td>
<td>-</td>
<td>0.032 (0.047)</td>
<td>-36.6 (10.6)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.892…</td>
<td>0.876 (0.499)</td>
<td>-</td>
<td>0.048 (0.101)</td>
<td>-49.8 (18.2)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.630…</td>
<td>-</td>
<td>0.922 (0.017)</td>
<td>0.018 (0.019)</td>
<td>-37.2 (7.5)</td>
<td></td>
</tr>
<tr>
<td>SC2</td>
<td>1.771…</td>
<td>-</td>
<td>0.648 (0.064)</td>
<td>0.022 (0.014)</td>
<td>-33.0 (5.1)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.892…</td>
<td>-</td>
<td>0.418 (0.177)</td>
<td>0.032 (0.017)</td>
<td>-32.9 (10.1)</td>
<td></td>
</tr>
</tbody>
</table>
Table 1.2. Example calculation of $P_i$ values for simulated water retention data from realization #1 of a $b = 3$, $j = 5$, $D = 1.771$…random Sierpinski carpet

<table>
<thead>
<tr>
<th>$I$</th>
<th>$N_p^{(i)}/b^{2i}$</th>
<th>$\theta_i$</th>
<th>$\theta_{i-1} - \theta_i$</th>
<th>$\sum_{n=1}^{i} N_p^{(n)}/b^{2n} \prod_{k=n}^{i-1} (1 - P_k)$</th>
<th>$P_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0.715</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>1</td>
<td>0.222</td>
<td>0.493</td>
<td>0.222</td>
<td>0.222</td>
<td>$P_1 = 1.000$</td>
</tr>
<tr>
<td>2</td>
<td>0.173</td>
<td>0.419</td>
<td>0.074</td>
<td>0.173</td>
<td>$P_2 = 0.428$</td>
</tr>
<tr>
<td>3</td>
<td>0.134</td>
<td>0.367</td>
<td>0.052</td>
<td>0.233</td>
<td>$P_3 = 0.223$</td>
</tr>
<tr>
<td>4</td>
<td>0.105</td>
<td>0.340</td>
<td>0.027</td>
<td>0.286</td>
<td>$P_4 = 0.094$</td>
</tr>
<tr>
<td>5</td>
<td>0.081</td>
<td>0.313</td>
<td>0.027</td>
<td>0.340</td>
<td>$P_5 = 0.079$</td>
</tr>
</tbody>
</table>
Figure 1.1. Example realizations for a) GM, b) SC1, and c) SC2 in a $b = 3$, $j = 2$, $D = 1.771\ldots$, random Sierpinski carpet with $D_d = 1.630\ldots$, and $P = 0.5$ (black = solid, white = air-filled pore, and grey = water-filled pore).
Figure 1.2. Sensitivity of the general scale-variant drainage model (GM) to the parameters $P$ and $D_d$.
Figure 1.3. Comparison of the different water retention models for the realizations giving the maximum difference in ESS between GM and SC1 (a, c and e) and between GM and SC2 (b, d and f) for D=1.630…, D=1.771… and D=1.892…. (b=3, j=5).
Figure 1.4. Mean values of $P_i$ calculated inversely from Eq. (16) as function of suction level. The error bars indicate one standard deviation around the mean.
Figure 1.5. Comparison of predicted relationships (lines) using mean parameter estimates from Table 1 in Eq. (3) with the observed values of $N_d$ (circles) calculated inversely from the simulated data. The error bars indicate one standard deviation around the mean.
PART II
ANALYTICAL PREDICTIONS AND LATTICE BOLTZMANN SIMULATIONS OF INTRINSIC PERMEABILITY FOR MASS FRACTAL POROUS MEDIA
Abstract

We present new analytical expressions, taking into consideration the size distribution and connectivity of pores, for the intrinsic permeability ($k$) of fractal porous media. The Menger Sponge is a three-dimensional mass fractal that provides a realistic representation of the complicated pore space geometry of soil and rock. Predictions based on the analytical models are compared with estimates of $k$ derived from lattice Boltzmann method (LBM) simulations of saturated flow in virtual representations of classical (deterministic) and randomized Menger Sponges. Overall, the analytically predicted $k$ values matched the $k$ values from the LBM simulations with < 14% error for deterministic sponges with minimum pore sizes ranging from 1/3$^1$ to 1/3$^4$. The differences generally diminished with decreasing Reynolds number (Re) (e.g., for a minimum pore size of 1/3$^3$, the error decreased from 11% at Re=0.40 to 1.6% at Re=0.07). Theoretical and empirical analyses of the surface fractal dimension ($D_2$) for successive slices through a random Menger Sponge show that the mean $D_2$ value, $\langle D_2 \rangle$, is equal to $D_3 - 1$, where $D_3$ is the 3-dimensional mass fractal dimension. This result also implies that the mean areal porosity is equal to volumetric porosity. Incorporating $\langle D_2 \rangle$ into Marshall’s probabilistic surface matching approach resulted in a $k = 3.27 \times 10^{-4}$ cm$^2$ for a random sponge with a minimum pore size of 1/3$^3$. This value compared favorably with the modal value of $k$ (=2.35x10$^{-4}$ cm$^2$) from LBM simulations performed in 100 realizations of this sponge. The proposed analytical model allows for the possibility of estimating $k$ from box counting analyses performed on digitized thin section images of natural porous media.
1. Introduction

Since the introduction of fractals as new geometric models for natural objects, numerous efforts have been made to harness their mathematics for challenging outstanding problems in hydrology. Fractals are inherently scaling. Thus, with the current interest in upscaling hydraulic properties, fractal models are being re-examined as viable descriptors of soils, aquifers, and reservoir rocks. Several theoretical investigations of the intrinsic permeabilities of fractal porous media have been presented over the past few decades. These are discussed below as a preface to the derivation of two new analytical models based on the well-known Menger Sponge fractal.

Early studies attempted to formulate expressions for the permeability based on the Kozeny-Carman (K-C) equation. The results suggested a general relationship between intrinsic permeability \( k \) and porosity \( \phi \) of the form: \( k \propto \phi^{\lambda} \), where \( \lambda \) is a scaling exponent. Different authors found varying expressions for the exponent \( \lambda \) as function of the pore or mass fractal dimension (e.g., Jacquin and Adler, 1987; Muller and McCauley, 1992). Gimenez et al. (1997) reviewed this research and developed their own intrinsic permeability model incorporating the effects of tortuosity and connectivity into the exponent \( \lambda \).

Adler and Thovert (1993) performed extensive numerical experiments by solving the Navier-Stokes equations for flow in one-, two-, and three-dimensional fractal structures. Their results were consistent with a generalized K-C equation for one-dimensional flow in a “stretched” Sierpinski Carpet. However, the scaling relationship between \( k \) and \( \phi \) turned out to be unreliable for two- and three-dimensional deterministic and random fractal porous media.
More recently, Yu and Liu (2004) developed a fractal model for $k$ by assuming continuous fractal pore-size and pore-length distributions based on Poiseulle’s equation. Xu et al. (2006a) developed tortuosity and permeability models for flow through a fractal-like tree network between one point and a straight line. The effective permeability of this network was obtained both in parallel and in series using Poiseuille’s equation including the effect of tortuosity. Xu et al. (2006b) extended this approach to find the permeability of a fractal disk-shaped network.

Following a different line of attack, Hunt (2001) employed continuum percolation theory to find the volume fraction of continuously distributed pores whose sizes are greater than or equal to a critical pore radius. The critical value, or the smallest pore in a connected network, was then related to the permeability based on an analogy between the Poiseuille and Darcy equations. This analysis, like most of those discussed previously, assumes all of the pores are interconnected. It does not take into account the presence of disconnected pores which do not contribute to flow. Since disconnected pores can occur in natural porous media, the ability of such fully-connected fractal models to accurately predict the $k$ of real soils and rocks is not clear.

Rawls et al. (1993) attempted to deal with the issue of disconnected pores by combining Marshall’s (1958) probabilistic approach with the fractal properties of a Sierpinski Carpet. In the Marshall (1958) model, two surfaces, each of which consists of $n$ sections, are exposed along a cut through an isotropic porous medium and then rejoined randomly. The surfaces are connected through necks which are assumed to be equal in size to the smallest mean pore area between any two contacting pores. Each $n$ section is assumed to have the same fraction of pore area, which is defined as the areal porosity.
The $n$ classes of pore cross-sections are denoted by a sequence of mean radii as $r_1, r_2, \ldots, r_n$. The average area of the pore necks is then calculated and related to $k$, i.e.

$$k = C \frac{\phi^a}{n^2} \sum_{i=1}^{l} 2(l - i) r_i^2$$  \hspace{1cm} (1)$$

where $C$ is a constant that depends on the pore geometry, $l$ is the number of pore classes up to $n$, and $a$ is a correction factor introduced later by Millington and Quirk (1960). In Marshall’s (1958) original paper $a$ was two. Rawls et al. (1993) modified Eq. (1) for fractal structures by replacing $r_i$ with $r_0/b^i$ and obtained,

$$k = C \phi^a \frac{r_0^2}{n^2}$$  \hspace{1cm} (2)$$

where $r_0$ is the width of the Sierpinski Carpet, $b$ is the scaling factor, and $r_1$ is the largest equivalent pore radius. Eq. (2) assumes that each pore size $r_i$ has the same fractional area. However, this is not realistic for a fractal structure. When two surfaces from a cross section through a fractal porous medium are rejoined randomly, as in the original Marshall approach, there will be different pore sizes with different fractional areas as opposed to the assumption of a constant fraction of pores. Thus, statistically matching two randomized fractal carpet surfaces will result in a different formulation from Eq. (2).

In this study, we present new analytical expressions for the intrinsic (saturated) permeability by employing a probabilistic model based on the connectivity of pores and Marshall’s (1958) approach. We test these models using lattice Boltzmann method (LBM) simulations performed in well-defined, explicit fractal structures (i.e., deterministic and random Menger Sponges).

2. Properties of Deterministic and Randomized Menger Sponges
The Menger sponge is a three-dimensional mass fractal with the capability of simulating a wide range of pore sizes and configurations. It is named after the mathematician Karl Menger (Mandelbrot, 1982). The Menger Sponge fractal has long been used as a well-defined prototype for natural porous media and employed as a model substrate for simulating flow and transport problems in complex pore space geometries (e.g., Garrison et al., 1992; Garza-López et al, 2000; Cihan et al., 2007).

The Menger Sponge is constructed from a solid initiator cube (embedding dimension $E = 3$) of unit length by an iterative process of mass removal and re-scaling. A generator is defined by sub-dividing the initiator into $b^E = 27$ smaller cubes of length $l = 1/b = 1/3$, and removing $m = 7$ of these. In the classical (deterministic) Menger Sponge, six of the removed cubes are central to the 6 faces of the initiator, while the remaining removed cube comes from the center of the initiator (Figure 2.1a). In a random Menger Sponge, the seven removed cubes are randomly chosen from the 27 solid cubes of length $1/b$ (Figure 2.1b). Construction continues by repeatedly applying the generator to the remaining solid cubes. Note that $l$ depends on $b$ as $l = 1/b^i$, where $i = 0, 1, 2, 3...$ is the level of iteration of the fractal algorithm. The number of solid cubes of length $l$, $N_{s3}(l)$, at the first iteration is $N_{s3}(1/3) = 20$. At the second iteration $N_{s3}(1/9) = 400$, and so on. In general, we have $N_{sE}(1/b^i) = b^{iD_E}$ where $D_E$ is the mass fractal dimension defined by the ratio $\log(b^E - m)/\log(b)$, with $m$ being the number of cubes removed in the generator.

The number of pores, $N_{pE}$, of length $l$ is given by,

$$N_{pE}^{(i)} = n_p b^{(i-1)D_E} = \left(b^E - b^{D_E}\right)b^{(i-1)D_E}$$

where $n_p$ is the number of pores in the generator, which is equal to $m = 7$ for the Menger Sponge. The porosity at any iteration level, $n$, is formulated by
\[\phi_k = \sum_{i=1}^{n} \frac{N^{(i)}_{n}}{b^{n \phi}} = 1 - b^{n(D_k - E)}\]  

where \(E = 3\) for the volumetric porosity of the Menger Sponge.

Figure 2.1 shows a deterministic Menger Sponge, and an example realization of a random Menger Sponge, iterated up to \(n = 3\) with \(b = 3\) and \(D_3 = 2.726\ldots\). The surface fractal dimensions \((D_2)\) of both structures change with distance (or slice number = \(b'\)) as one moves from one face through the interior to the opposite face. Figure 2.2 shows the variation in \(D_2\) as a function of slice number for both deterministic and random Menger Sponges. The maximum value of \(D_2\) inside the deterministic Menger Sponge is 1.892\ldots which is the fractal dimension of the Sierpinski Carpet; the minimum value of \(D_2 = 1.261\ldots\) occurs in the middle of the deterministic sponge.

Surface fractal dimensions of the slices inside a randomized Menger Sponge change for each realization of the sponge due to the randomization process. Figure 2.2 shows changes in \(D_2\) with slice number for one example realization of a random Menger Sponge. Figure 2.2 also shows changes in the mean value of \(D_2\) for each slice based on 100 random realizations. The line is almost invariant and indicates that \(\langle D_2 \rangle \approx D_3 - 1\), where \(\langle D_2 \rangle\) is the mean value. A formal proof of this result is given below.

For the sake of simplicity, we will only consider the first iteration level since it will be sufficient to deduce information about the relationship between \(\langle D_2 \rangle\) and \(D_3\). At \(i = 1\), the number of boxes (either solid or pore), \(n_{b}^{(1)}\), in each slice is equal to \(b^2\). The number of solids inside the Menger Sponge generator as a whole is given by \(b^{D_0}\) and the probability or proportion of \(1/b^1\) sized solids, \(p_1\), in the whole system is \(b^{D_0} / b^3\). The probability of obtaining \(x_1\) number of \(1/b^1\) sized solids from a random slice with \(b^2\) boxes
through this structure when sampling without replacement can be calculated from the hypergeometric distribution. The expected value of \( x_1 \) from the hypergeometric distribution is given by \( \langle x_1 \rangle = n_b^{(i)} p_i = b^{(D_3 - 1)} \). Then, by definition, the mean surface fractal dimension of multiple slices through a single randomized Menger Sponge (or single slices through multiple random realizations) must be:

\[
\langle D_3 \rangle = \frac{\log \langle x_1 \rangle}{\log b} = D_3 - 1
\]

(5)

which explains the observed behavior in Figure 2.2. According to the definition of porosity given by Eq. (4), Figure 2.2 and Eq. (5) imply that \( \langle \phi_2 \rangle = \phi_3 \), i.e., the mean areal porosity is equal to the volumetric porosity. This is a convenient assumption commonly employed in subsurface hydrology.

The scaling factor \( b \) represents the length ratio of the initiator relative to the largest pore present, and thus could be estimated from the air entry value and sample dimensions for a given porous medium. Finer textured or clay-rich soils can be expected to exhibit larger \( b \) values as compared to coarser soils (Brakensiek and Rawls, 1992).

Gibson et al. (2006) report independent estimates of \( b \) and \( D_E \) for soil aggregates based on image analysis and density scaling of two- and three-dimensional computed tomographic scans. The values of \( b \) and \( D_3 \) ranged from 4 to 15 and from 2.97 to 2.99, respectively. Their results also indicate that \( \langle D_2 \rangle \cong D_3 - 1 \).

3. Analytical Models for Intrinsic Permeability

Neglecting inertial effects, the mean velocity of a fluid, \( u \), in a narrow tube of radius, \( r_t \), is given by the Poiseuille equation, i.e.
\[ u = -\frac{C r_i^2 \, dh}{\mu \, dl} \]  

(6)

where \( C \) is a shape factor, \( \mu \) is the dynamic viscosity (Pa s), and \( dh/dl \) is the potential gradient driving the fluid flow in the tube. If the porous medium is considered to be made up of channels of different sizes, Poiseuille’s equation is analogous to Darcy’s law, which expresses the mean velocity of a fluid in a porous medium, and can be written as:

\[ q = -\frac{k \, dh}{\mu \, dl} \]  

(7)

where \( k \) is equivalent to \( \langle C r_i^2 \rangle \), which is an averaged quantity for a porous medium. The shape factor \( C \), changes depending on the geometry of the pore. Its value is equal to 1/8 for circular pores. Pores in the Menger Sponge are square, however, and flow is assumed to be in the z direction. Neglecting inertial and end effects, and assuming no interaction between adjacent pores (pores are assumed to be surrounded with solid boundaries where a no-slip boundary condition applies at the walls of a square), the solution of the Navier-Stokes equation for the average velocity within an individual square pore is given by (Papanastasiou et al., 2000):

\[ u_i = -C \frac{d_i^2}{\mu} \frac{dh}{dz} ; \quad C = \frac{1}{12} \left[ 1 - 6 \sum_{k=0}^{\infty} \frac{\tanh \left[ \pi \left( k - 1/2 \right) \right]}{\pi^5 \left( k - 1/2 \right)^5} \right] \approx 0.035 \]  

(8)

where \( d \) is the side length of the pore. The area of pores at the \( i \)-th iteration level of the Menger Sponge algorithm can be written as \( d_i^2 = r_0^2 / (b_i^2) \) where \( r_0 \) is the width of the sponge.
3.1. Probabilistic Capillary-Connectivity (PCC) Model

The method employed here separates the system into different connected flow paths or networks. Consider a network consisting of only the largest pores of size $r_0/b$ connected from one end to the other in the direction of flow. According to Poiseuille’s equation, the mean velocity of water following such a pathway is proportional to $r_0^2/b^2$.

We define a probability for the existence of such a network as $P_1 N_{p3}^{(1)} / b^3$, where $N_{p3}^{(1)} / b^3$ is the proportion of the largest pores in the whole volume and $P_1$ represents the proportion of pores of size of $r_0/b$ connected from one end to the other. The remaining proportion of pores of size $r_0/b$ is given by $(1 - P_1) N_{p3}^{(1)} / b^3$; these pores may be completely unconnected or connected with smaller pores of size $r_0/b^2$ to form a different flow pathway. There might also be a network formed by only the $r_0/b^2$-sized pores. The probability for the existence of a network containing $r_0/b^2$-sized pores or $r_0/b$- and $r_0/b^2$-sized pores is written as $P_2 (N_{p3}^{(2)} / b^{2+3} + (1 - P_1) N_{p3}^{(1)} / b^3)$ where $P_2$ represents the connected proportion of pores in networks formed by $r_0/b^2$- or larger-sized pores. Since flow is controlled by the smallest pores within a network of different-sized connected pores, the mean velocity of water following a pathway consisting of $r_0/b$- and $r_0/b^2$-sized pores is assumed to be proportional to area of the smaller pores, i.e. $r_0/b^2$. In generalized form, the pore areas controlling flow in the different flow paths, multiplied by their associated probabilities, are written as:
\[ i = 1 \quad P_1 \frac{N_{\rho E}^{(i)} r_0^2}{b^E} \]

\[ i = 2 \quad P_2 \left[ \frac{N_{\rho E}^{(2)} r_0^2}{b^{2E}} + (1 - P_1) \frac{N_{\rho E}^{(1)} r_0^2}{b^E} \right] \]

\[ i = 3 \quad P_3 \left[ \frac{N_{\rho E}^{(2)} r_0^2}{b^{3E}} + (1 - P_2) \frac{N_{\rho E}^{(2)} r_0^2}{b^{2E}} + (1 - P_2)(1 - P_1) \frac{N_{\rho E}^{(1)} r_0^2}{b^E} \right] \]

\[ \vdots \quad \vdots \]

\[ i = n \quad P_n \left[ \frac{N_{\rho E}^{(n)} r_0^2}{b^{nE}} + (1 - P_{n-1}) \frac{N_{\rho E}^{(n-1)} r_0^2}{b^{n-1E}} + \cdots + (1 - P_{n-1})(1 - P_{n-2}) \cdots (1 - P_1) \frac{N_{\rho E}^{(1)} r_0^2}{b^E} \right] \]

(9)

Permeability is defined by the expected value, \( \langle C r_i^2 \rangle \), i.e. the summation of all the terms above leading to;

\[ k(n) = C r_0^2 \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{N_{\rho E}^{(i)} P_j}{b^{iE}} \frac{P_j}{b^{2j}} \prod_{k=i}^{j-1} (1 - P_k) \]

(10)

where \( n \) is the last iteration level of the fractal porous medium, and the pore shape factor \( C \) is assumed to be constant for all pores. Summation of the probabilities yields the connected proportion of pores in the flow system and is equivalent to the effective porosity \( \phi_{\text{eff},E} \), i.e.

\[ \phi_{\text{eff},E}(n) = \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{N_{\rho E}^{(i)} P_j}{b^{iE}} \prod_{k=i}^{j-1} (1 - P_k) \]

(11)

Cihan et al. (2007) used a similar approach to the above in their analysis of scale-variant fractal water retention functions during monotonic drainage. The different \( P_i \) values in Cihan et al. (2007) indicated the connected proportions of water-filled pores at different suction levels and were named the probability of drainage. Here, since all the pores are filled with water, each \( P_i \) value represents the proportion of connected pores whose sizes are greater than or equal to \( 1/b^i \). When \( P_i \to 1 \) the system approximates a
“stretched” Sierpinski Carpet. Now if we consider a steady flow field created in a deterministic Menger Sponge by a pressure gradient in one direction (constant pressure boundary conditions are applied on two opposing faces, and the rest are assigned to be no flow boundary conditions), the proportion of the largest pores of size $r_0/b$ connected from one end to the other in the direction of the flow, $P_1$ is equal to $3/7$. The same statistics apply for $r_0/b^2$-sized pores connected from one end to the other in the direction of the flow because $3/7$ of these pores are connected to the remaining $4/7$ of the $r_0/b$-sized pores, i.e., $P_2 = P_1 = 3/7$.

Assuming that all of the probabilities are constant and equal, i.e., $P = P_1 = P_2 = \ldots = P_n$, evaluation of the series for $E = 3$ in Eqs. (10) and (11) renders

\[
k(n) = C r_0^2 \frac{P(b^3 - b^{D_3})}{P-1+b^2} \left[ \frac{(1-P)^{(D_3-3)logb} - (1-\phi_3)}{b^{D_3} + b^3(P-1)} - \frac{(1-P)}{(1-\phi_3)^{(D_3-3)}} + b^2 \frac{1-(1-\phi_3)^{(D_3-5)}}{b^5 - b^{D_3}} \right] \tag{12}
\]

\[
\phi_{eff}^3(n) = \phi_3 - \left( \frac{b^3 - b^{D_3}}{b^{D_3} + b^3(P-1)} \right)^{(1-P)^{(D_3-3)logb} + (1-\phi_3)} \tag{13}
\]

where $\phi_3 = 1 - (b^n)^{(D_3-3)}$ is the total porosity. Since the $P$ values in Eqs. (10)-(13) are allowed to vary with direction, the above expressions can also be written in tensor form for applications in anisotropic systems.

Variation of the effective porosity with the total porosity for various $P$ values is presented in Figure 2.3(a). This figure shows that as the connectivity of the system measured with $P$ decreases, the effective porosity decreases compared to the porosity. Changes in the permeability as a function of porosity are shown for various $P$, $b$, and $D_3$ values in Figures 2.3(b)-(d). The permeability decreases with decreasing $P$. When $P=0,$
the system is below the percolation threshold, and the permeability is zero. Figures 2.3(c) and 2.3(d) indicate that the permeability appears to be much more sensitive to $b$ than $D_3$.

As $n$ approaches infinity, Eq. (13) approaches unity, and Eq. (12) reduces to:

$$k = C r_0^2 \frac{P b^2 (b^3 - b^{D_3})}{(P-1+b^2)(b^5 - b^{D_3})}$$

(14)

From the above discussion, a $P$ value of 3/7 can be used in Eqs. (12) and (14) for the prediction of the intrinsic permeability of a deterministic Menger Sponge. Since the $P$’s are not necessarily equal in a random Menger Sponge due to the randomization process, forward prediction by applying Eqs. (12) or (14) to random structures may not be possible. For random Menger Sponges, $P$ is assumed to be a constant parameter, equivalent to a measure of connectivity that can be estimated inversely by comparison with experimental or numerical simulation results. For forward prediction of intrinsic permeability in the case of random Menger Sponges, Marshall’s probabilistic approach can be followed.

3.2. Marshall’s Probabilistic Approach (MPA)

Following an approach similar to Marshall (1958), two surfaces from a cross-sectional cut through a random Menger Sponge are rejoined randomly (Figure 2.4). The surfaces are connected through pore necks, whose sizes are assumed to be the intersection areas between pairs of contacting pores. Table 1 shows an example of the calculation of probabilities of possible pore neck areas that result from matching of two randomized unit fractal faces at the second iteration level. Each fractal face has the same fractal dimension, $D_2 = \log 7/\log 3$. The width of the largest pores is 1/3 and the areal fraction of the largest pores is 2/9. The width of the smallest pores with areal fraction of 14/81 is
$1/3^2$ (Table 1). Matching these two faces may result in two possible pore neck areas. One possibility for any given realization of the faces is that the largest pores on one face can match with those on the other face, which results in a pore neck area of $1/3^2$. The other possibility is the $1/3^4$ pore neck area that might result from intersecting a $1/3$ with $1/3^2$ pore or a $1/3^2$ with $1/3^2$ pore width on one face with the other. Since the randomization of the faces associated with the same fractal dimension are assumed to be independent events, the probability of $1/3^2$ pore neck area can be calculated by multiplying the areal fraction of pores of $1/3$ width in the two faces, i.e. $p(1/3^2) \cap p(1/3^2) = 2/9 \times 2/9 = 4/81$. Likewise, the probability of $1/3^4$ pore neck area can be calculated by taking into account all possible pore pairs that give $1/3^4$ neck area, i.e., $p(1/3^4) \cap p(1/3^4) + 2x[p(1/3^2) \cap p(1/3^4)]$. The second term is multiplied by two because as the pores of $1/3$ width in the first face may intersect with the pores of $1/3^2$ width in the second face, the pores of $1/3$ width present in the second face may also intersect with the pores of $1/3^2$ width in the first face, which result in a $1/3^4$ pore neck area.

Generalization of the above procedures to matching of any arbitrary two faces with the same arbitrary fractal dimension is as follows. The areal fraction of pores of size of $1/b$ is equal to $p(1/b^2) = N_{p2}^{(i)} / b^2$, where $N_{p2}^{(i)}$ is the number of pores generated at first iteration level of a slice ($E = 2$) in a fractal porous medium. The probability of occurrence for the solid space area is equal to $1 - \phi^2_s$. The probability of occurrence of $1/b^2$ neck areas resulting from the intersection of pores with $1/b$ width on one surface with pores of $1/b$ width on the other surface can be evaluated as $p(1/b^2) \cap p(1/b^2) = (N_{p2}^{(i)} / b^2)^2$. Likewise, the probability of occurrence of $(1/b^2)^2$ neck areas resulting from the intersection of pairs of pores $1/b^2 - 1/b^2$ and $1/b - 1/b^2$ on the matching surfaces can be written.
as \((N^{(2)}_{p2}/b^4)^2 + 2 \times (N^{(2)}_{p2}/b^2 \times N^{(2)}_{p2}/b^4)\). The probabilities for all possible neck areas are given in Table 2.

According to the axiom of probability, summation of the probabilities must equal unity, i.e.

\[
\sum P_i = 1 - \phi^2 + \left[ \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{N^{(i)}_{p2} N^{(j)}_{p2}}{b^{2i} b^{2j}} + \sum_{i=2}^{n-1} \sum_{j=1}^{n} \frac{N^{(i)}_{p2} N^{(j)}_{p2}}{b^{2i} b^{2j}} \right] = 1
\]  

The term in the brackets of Eq. (15) is a symbolic representation for the summation of the probabilities in Table 1 excluding the probability of the zero neck area, \(1 - \phi^2\). The term in the brackets can be shown to be equal to \([1 - b^{(D_2-2)}]^2 = \phi^2\) by evaluating the series after substitution of \(N^{(i)}_{p2} = \left(b^2 - b^{D_2}\right)b^{D_2-i}\). Multiplying probable neck areas with the probabilities and summing over all sizes, we obtain the total expected area, \(\left\langle r^{2}_i \right\rangle\), which can be written in symbolic form as,

\[
\left\langle r^{2}_i \right\rangle = r_0^2 \left[ \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{N^{(i)}_{p2} N^{(j)}_{p2}}{b^{2i} b^{2j}} \left( \frac{1}{b^i} \right)^2 + \sum_{i=2}^{n-1} \sum_{j=1}^{n} \frac{N^{(i)}_{p2} N^{(j)}_{p2}}{b^{2i} b^{2j}} \left( \frac{1}{b^i} \right)^2 \right]
\]  

where \(r_0\) is the characteristic length of the porous medium that shows fractal behavior.

Recalling the definition of \(k\) previously given and invoking the relationship \(<D_2> = D_2 - 1\), we can formulate the permeability of a random Menger Sponge by evaluating the series in Eq. (16) as:

\[
k(n) = C r_0^2 \left[ \frac{\left(b^2 - b^{(D_2)}\right)^2 \left(b^4 + b^{(D_2)}\right)}{\left(b^4 - b^{(D_2)}\right)\left(b^6 - b^{2(D_2)}\right)} - 2 \frac{\left(b^2 - b^{(D_2)}\right)}{\left(b^4 - b^{(D_2)}\right)\left(b^6 - b^{2(D_2)}\right)} \left(1 - \left\langle \phi_2 \right\rangle\right) \frac{\left(D_2\right)^{-4}}{\left(D_2\right)^{-2}} + \frac{\left(b^4 - b^{2(D_2)}\right)}{\left(b^6 - b^{2(D_2)}\right)\left(1 - \left\langle \phi_2 \right\rangle\right)^{\left(D_2\right)^{-6}}} \right]
\]  

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where \( \langle \phi_2 \rangle = 1 - (b^n)^{\langle D_2 \rangle - 2} \).

The variation of \( k \) with porosity predicted by Eq. (17) is shown in Figure 2.5. The MPA model shows a very similar behavior to the PCC model for the different values of \( b \) and \( \langle D_2 \rangle \). Likewise, the permeability appears to be more sensitive to \( b \) than \( D_2 \). However, the application of the MPA model is limited to more or less isotropic porous media since the mean surface fractal dimension \( \langle D_2 \rangle \) is representative for the whole structure, while the variation of \( k \) along different directions in anisotropic systems can only be taken into account by the PCC model.

Except for very low values of \( b \), the series converges very quickly. Eq. (17) can then be simplified by allowing \( n \to \infty \), i.e.

\[
k = C r_0^2 \frac{(b^n - b^{\langle D_2 \rangle})^2 (b^4 + b^{\langle D_2 \rangle})}{(b^4 - b^{\langle D_2 \rangle})(b^6 - b^{2\langle D_2 \rangle})} \tag{18}
\]

4. The Lattice Boltzmann Method (LBM)

Detailed introductions to the LBM can be found in Sukop and Thorne (2006), Succi (2001), and Wolf-Gladrow (2000). In this section we provide a brief summary of the 3-D LBM to numerically compute the permeability of the deterministic and random Menger Sponges. This single phase fluid flow problem is among the simplest capabilities of the LBM and the current work can be viewed as a prelude to future efforts that will consider unsaturated flows. We use the simplest Bhatnagar-Gross-Krook (BGK) single relaxation time model in this work. The BGK model is known to have limitations (Pan et al., 2006), but careful application gives adequate results in many applications.
Here, we have implemented the LBM in three dimensions for a single component system. The distribution function $f$ represents a fluid and satisfies the following LB equation:

$$f_a(x + e_a \Delta t, t + \Delta t) = f_a(x, t) - \frac{\Delta t}{\tau} \left( f_a(x, t) - f_a^{eq}(x, t) \right), \quad (19)$$

where $f_a(x, t)$ is the density distribution function in the $a$-th velocity direction, $\tau$ is a relaxation time that is related to the kinematic viscosity through $\nu = c_s^2 (\tau - 0.5 \Delta t)$, $e_a$’s are the discrete velocities, and $w_a$’s are the direction-specific weights. The equilibrium distribution function $f_a^{eq}(x, t)$ can be calculated as

$$f_a^{eq}(x, t) = w_a \rho \left[ 1 + \frac{e_a \cdot u}{c_s^2} + \frac{(e_a \cdot u)^2}{2c_s^4} - \frac{u^2}{2c_s^2} \right]. \quad (20)$$

where $\rho$ is the density of the fluid, which can be obtained from $\rho = \sum_{a=0}^{18} f_a$ and $u$ is the velocity of the fluid. For the D3Q19 model, the discrete velocities are given by,

$$\begin{bmatrix} e_0, e_1, e_2, e_3, e_4, e_5, e_6, e_7, e_8, e_9, e_{10}, e_{11}, e_{12}, e_{13}, e_{14}, e_{15}, e_{16}, e_{17}, e_{18} \end{bmatrix} = c_s \cdot \begin{bmatrix} 0 & 1 & -1 & 0 & 0 & 0 & 0 & 1 & 1 & -1 & 1 & -1 & 1 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 1 & 1 & -1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 \end{bmatrix}.$$

$w_a = 1/3 \quad (a = 0), \quad w_a = 1/18, \quad (a = 1, 2, \ldots, 6), \quad w_a = 1/36, \quad (a = 7, 8, \ldots, 18)$, $c_s = c/\sqrt{3}$,

where $c_s = \Delta x / \Delta t$ is the ratio of lattice spacing $\Delta x$ and time step $\Delta t$. Here, we define 1 lattice unit ($\Delta x$) as 1 lu. The macroscopic momentum $\rho u$ is defined as:

$$\sum_{a=0}^{18} f_a e_a = \rho u. \quad (21)$$
Pressure is proportional to density in this model and the relationship – known as the Equation of State – is \( P = c_s^2 \rho \) or simply \( P = \frac{\rho}{3} \) for the model we employ here.

5. Results and Discussion

5.1. Deterministic Menger Sponge

We calculated the intrinsic permeability (\( k \)) as a function of maximum iteration level (\( n \)) for a deterministic Menger Sponge of unit (1 cm) width, with \( b = 3 \), and fractal dimension \( D_3 = 2.726 \) (Figure 2.1a). Based on this information and setting \( P = 3/7 \), Eq. (12) was used to estimate \( k \) for unidirectional, steady, laminar flow of a fluid passing through the deterministic sponge. Because flow is dominated by the largest pore, which occurs at \( n = 1 \), there was not much difference between the \( k \) values estimated by the probabilistic capillary-connectivity (PCC) model as a function of maximum iteration level (Table 3). Going from \( n = 1 \) to \( n = 4 \), the intrinsic permeability increases by \(~16\%)\.

The limiting form of the permeability given by Eq. (14) results in a \( k \) value differing less than 0.15\% from that given by Eq. (12) for the deterministic Menger Sponge with \( n > 2 \). The ratio of the effective porosity to the total porosity varies between 0.42 and 0.76 from \( n=1 \) to \( n=4 \).

We also evaluated the intrinsic permeability of the deterministic Menger Sponge illustrated in Figure 2.1(a) using the LBM. We simulated flow at different levels of construction up to \( n = 4 \). The simulations use periodic boundaries on the sides of the domain (so the opposite sides are effectively connected) and pressure boundaries on the top and bottom that impose a gradient across the fractal domain. The pressure distribution occurring across the sponge is shown from a slice of the simulation domain in a Menger
Sponge with \( n = 3 \) (Figure 2.6). In a convenient form for the LBM, Darcy’s law, Eq. (7), is

\[
q = \frac{k}{\rho c_s^2 (\tau - 0.5) \Delta t} \frac{\Delta p}{L},
\]

where \( q \) is the Darcy flux (the average velocity of fluid exiting the entire face – including solid areas where the velocity is zero), \( c_s^2 (\tau - 0.5) \) is the kinematic viscosity, and \( \Delta p/L \) is the pressure gradient. Note that the average fluid density is used in the denominator of Eq. (22).

Here we provide a brief description of the calculation of intrinsic permeability and Reynolds numbers for the LBM measurements. For all cases in Table 3, the domain was \( 243 \times 243 \times 243 \) lu\(^3\). Fluid densities of 1.005 and 0.995 mu lu\(^{-3}\) were applied to the ends of the model domains. This gives an average density of 1 mu lu\(^{-3}\) and corresponding inlet and outlet pressures of \( p_{in} = 0.335 \) and \( p_{out} = 0.3316 \) mu lu\(^{-1}\)ts\(^{-2}\), respectively. For the \( i = 3 \) sponge under those conditions, the observed flow through the system was about 16.25 lu\(^3\)ts\(^{-1}\). The corresponding Darcy flux \( q \) is the flow divided by the cross-sectional area or \( q = 16.25 \) lu\(^3\)ts\(^{-1}\)/(243 \times 243 \) lu\(^2\) = 2.75\times10^{-4} \) lu ts\(^{-1}\). Solving (22) for permeability \( k \), we get \( k = 33.4 \) lu\(^2\). Conversion to real units involves multiplication by the scale conversion factor as follows:

\[
k(\text{physical}) = k(\text{LBM}) \left( \frac{L_{\text{physical}}}{L_{\text{LBM}}} \right)^2 \tag{23}
\]

where the \( L \)'s are the length of any comparable feature in physical and LBM units.
We computed the average Reynolds Numbers $\text{Re} = \bar{u} L / \nu$ where $\bar{u}$ is the mean pore velocity $(q/\phi_3)$, and $\nu$ is the dynamic viscosity of water. The Reynolds number increased slightly with iteration level of the structure under a constant pressure gradient (Table 3). We computed a second $k$ value for the deterministic structure at $i=3$ while decreasing the pressure gradient. When $\text{Re}=0.40$ for a 1 cm sponge, the LBM $k$ value for $i = 3$ is $5.66 \times 10^{-4}$ cm$^2$. For $\text{Re} = 0.07$ where departure from Darcy’s law behavior should be very small, the LBM $k$ value reduced to $5.12 \times 10^{-4}$ cm$^2$, which compares very favorably to the $k$-PCC, $5.04 \times 10^{-4}$ cm$^2$, predicted by our new analytical expression (12), which ignores inertial and end effects.

We also computed the permeability of the stretched Sierpinski carpet ($b=3$, $D_3=\log 24/\log 3$, and $n=3$) using both Eq. (12) and the LBM. Setting $P=1$, Eq. (12) predicts a PCC–$k= 4.81 \times 10^{-4}$ cm$^2$. The corresponding LBM–$k$ for the stretched Sierpinski carpet is $4.32 \times 10^{-4}$ cm$^2$.

### 5.2. Random Menger Sponge

The $P$-value in the PCC model was calculated to be 0.20 by equating Eq. (12) to the modal value of the LBM permeability from 100 realizations. This indicates that on the average, 20% of the pore volume, including the pores whose sizes are equal to or greater than $1/b^i$ ($i=1, 2, \text{and } 3$) can form a connected path from one end to the other. From Eq. (13), the mean effective porosity of the random Menger Sponges at $n = 3$ was estimated as 0.22, as compared to the total porosity of 0.594.

Based Eq. (17), and neglecting the effect of pore coalescence (i.e., assuming the shape factor, $C \sim 0.035$, does not change with the randomization), the MPA intrinsic permeability of a randomized Menger Sponge of 1 cm width, with $b = 3$, $n = 3$ and a
surface fractal dimension of $\langle D_n \rangle = 1.726$ is predicted to be $3.27 \times 10^{-4}$ cm$^2$. As expected, the intrinsic permeability of the random structure is less than that of the deterministic one (a 35% reduction in the case of $n = 3$). The $k$ is reduced because the randomization process interrupts the direct flow paths through the largest pores which increases the tortuosity, and disconnects and/or isolates many pores from the main flow paths which decreases the effective porosity.

We also computed $k$ using the LBM for 100 realizations of the $b = 3$, $D = 2.726\ldots$, and $n = 3$ randomized Menger Sponge generated using the homogenous algorithm (Sukop et al., 2001). These are the same parameters that characterize the deterministic structure in Figure 2.1(a), but the positions of the pores are allowed to vary randomly. Figure 2.1(b) shows one such realization. The distribution of the permeability values is presented in Figure 2.7. The distribution is strongly skewed towards the lower $k$ values. The modal value of the LBM permeability for the random Menger Sponge was equal to $2.35 \times 10^{-4}$ cm$^2$, which was approximately 54% lower than the permeability of the deterministic Menger Sponge. This value was very close to the predicted value of $k$ ($= 3.27 \times 10^{-4}$ cm$^2$) from the MPA analytical model.

6. Concluding Remarks

Applying Poiseuille’s equation and probabilistic approaches to deterministic and random Menger Sponges resulted in new analytical expressions to estimate the intrinsic (saturated) permeability of mass fractal porous media. The analytical model predictions compared favorably with the Lattice Boltzmann simulations for the intrinsic permeabilities of both deterministic and random Menger Sponges of a unit cm width,
with $b = 3$, $n = 3$ and $D = 2.726...$. The results showed that the intrinsic permeability of the random structure is less than that of the deterministic ones. The modal LBM permeability of 100 realizations of the random Menger Sponge was 54% lower than the permeability of the deterministic Menger Sponge. A similar trend was observed for the analytical models going from the deterministic to the random structure.

The theoretical and empirical analyses presented in this study suggest that the permeability might be predicted with the MPA model by estimating $b$ and $D_2$ from box counting analyses performed on digitized thin section images of natural porous media. However, the application of the MPA permeability model may not be reliable in highly anisotropic and heterogeneous porous media due to high variation in $D_2$ along the direction $k$ being measured. On the other hand, the PCC permeability model takes into account the anisotropy and heterogeneity but includes one additional variable $P$ that is a measure of connectivity. It may be possible to estimate the $P$ parameter inversely from water retention data using the model of Cihan et al. (2007).

We plan to extend the probabilistic and fractal approaches presented here to the derivation of relative permeability models for the case of unsaturated flow. Testing of new analytical models is achievable with a multiphase Lattice Boltzmann method (Huang et al., 2007) that is free of many of the assumptions commonly made when applying capillary theory to porous media.
LIST OF REFERENCES
References


APPENDIX
Table 2.1. Example calculation of probability of neck areas resulted from matching of two randomized faces with unit width. In the first row, only the pores shaded with red are taken into account to calculate probability of the neck area in the third column. In the second row, green phase indicates the pores contributing the calculation of probability of the neck area at the next level.

<table>
<thead>
<tr>
<th>Face 1</th>
<th>Face 2</th>
<th>Probable neck area</th>
<th>Probability</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1" alt="Face 1" /></td>
<td><img src="image2" alt="Face 2" /></td>
<td>$p\left(\frac{1}{3^2}\right)$</td>
<td>$p\left(\frac{1}{3^2}\right) \cap p\left(\frac{1}{3^2}\right) = \frac{2}{9} \times \frac{2}{9} = \frac{4}{81}$</td>
</tr>
<tr>
<td>$p\left(\frac{1}{3^2}\right) = \frac{2}{9}$</td>
<td>$p\left(\frac{1}{3^2}\right) = \frac{2}{9}$</td>
<td>$p\left(\frac{1}{3^4}\right) \cap p\left(\frac{1}{3^4}\right) + p\left(\frac{1}{3^2}\right) \cap p\left(\frac{1}{3^4}\right) + p\left(\frac{1}{3^4}\right) \cap p\left(\frac{1}{3^2}\right) = \left(\frac{14}{81}\right)^2 + 2 \times \frac{14}{81} \times \frac{2}{9} = \frac{700}{81^2}$</td>
<td></td>
</tr>
<tr>
<td>$p\left(\frac{1}{3^4}\right) = \frac{14}{81}$</td>
<td>$p\left(\frac{1}{3^4}\right) = \frac{14}{81}$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Note: $p(\cdot)$ indicates areal proportion of pores.
Table 2.2. Neck area vs. probability from the random intersection of two fractal surfaces.

<table>
<thead>
<tr>
<th>Probable Pore Neck Area</th>
<th>Probability</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$1 - \phi^2$</td>
</tr>
<tr>
<td>$(\frac{1}{b})^2$</td>
<td>$(\frac{N_p^{i=1}}{b^2})^2$</td>
</tr>
<tr>
<td>$(\frac{1}{b^2})^2$</td>
<td>$(\frac{N_p^{i=2}}{b^4})^2 + 2\left(\frac{N_p^{i=1}}{b^2} \times \frac{N_p^{i=2}}{b^4}\right)$</td>
</tr>
<tr>
<td>$(\frac{1}{b^3})^2$</td>
<td>$(\frac{N_p^{i=3}}{b^6})^2 + 2\left(\frac{N_p^{i=1}}{b^2} \times \frac{N_p^{i=3}}{b^6}\right) + 2\left(\frac{N_p^{i=2}}{b^4} \times \frac{N_p^{i=3}}{b^6}\right)$</td>
</tr>
<tr>
<td>:</td>
<td>:</td>
</tr>
</tbody>
</table>

Table 2.3. Comparison of the model results for the deterministic Menger Sponge

<table>
<thead>
<tr>
<th>$i$</th>
<th>$\phi_3$</th>
<th>$\phi_{eff}$</th>
<th>$k$-PCC $(x10^{-4}\text{cm}^2)$</th>
<th>$k$-LBM $(x10^{-4}\text{cm}^2)$</th>
<th>Re-LBM</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.26</td>
<td>0.11</td>
<td>4.34</td>
<td>5.02</td>
<td>0.36</td>
</tr>
<tr>
<td>2</td>
<td>0.45</td>
<td>0.26</td>
<td>4.97</td>
<td>5.53</td>
<td>0.39</td>
</tr>
<tr>
<td>3</td>
<td>0.59</td>
<td>0.40</td>
<td>5.04</td>
<td>5.66</td>
<td>0.40</td>
</tr>
<tr>
<td>4</td>
<td>0.70</td>
<td>0.53</td>
<td>5.05</td>
<td>5.73</td>
<td>0.41</td>
</tr>
</tbody>
</table>

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Figure 2.1. a) Deterministic Menger Sponge of unit width with $b = 3$, $n = 3$, a mass fractal dimension of $D_3 = \log_{20}/\log_3 = 2.726\ldots$ and $D_2 = \log_{8}/\log_3 = 1.892\ldots$ for each face of the cube, and b) one realization of a randomized Menger Sponge with unit width, with $b = 3$, $n = 3$, $D_3 = 2.726$, and $\langle D_2 \rangle = 1.726$. 
Figure 2.2. Variation of the fractal dimension $D_2$ through slices of deterministic and random Menger Sponges with $b = 3$, $n = 3$, and $D_3 = 2.726\ldots$
Figure 2.3. Variation of the PCC model effective porosity and intrinsic permeability with the model parameters: a) $\phi_{eff}$ versus $\phi_3$ as function of $P$, and $k_{PCC}$ versus $\phi_3$ as function of b) $P$, c) $D_3$ and d) $b$ ($r_0 = 1$ cm, $C = 0.035$).
Figure 2.4. Matching of two random fractal surfaces of the same $b$ and $D_2$ values (adapted from Hillel, 1998)
Figure 2.5. Variation of the MPA-intrinsic permeability with a) $D_2$ and b) $b$ ($r_0=1$ cm, $C' = 0.035$).
Figure 2.6. Vertical slices through the center of a Menger Sponge showing pressure distribution (left) and velocity vectors (right).
Figure 2.7. Distribution of k from LBM simulations in 100 realizations of the $b = 3$, $D = 2.726$, and $n = 3$ randomized Menger Sponge.
PART III
PREDICTING RELATIVE PERMEABILITY FROM WATER RETENTION: A DIRECT APPROACH BASED ON FRACTAL GEOMETRY
Abstract

Predicting a soil relative permeability curve from a fitted water retention curve with shared parameters avoids the timely and difficult measurement of the relative permeability curve. We present a new approach to predict relative permeability by direct use of measured soil water retention data without any fitting procedures. The new relative permeability model, derived from a probabilistic-fractal approach, appears in series form as a function of suction and the incremental change in water content. This discrete approach describes the drained pore space and permeability at different suctions incorporating the effects of both pore-size distribution and connectivity among water-filled pores. We compared the performance of the new model to predict of relative permeability to that of the van Genuchten-Mualem (VG-M) model for 35 paired data sets from the UNSODA database and five other previously published data sets. At the 5% level of significance, the new method predicts relative permeabilities from the UNSODA database significantly better (mean logarithmic root mean square error, LRMSE = 0.813) than the VG-M model (LRMSE = 1.555). Each prediction of relative permeability from the five previously published data sets were also significantly better.

1. Introduction

Knowledge of the unsaturated hydraulic conductivity or relative permeability is critical for describing the flow of fluids and solutes in the vadose zone. Solution of the partial differential equations governing the flow of fluids under variably-saturated conditions requires appropriate constitutive relationships among permeability, saturation, and capillary pressure.
Because measurement of relative permeability is difficult, attempts to predict this function from measurements of water retention have proliferated. Most attempts rely on, more or less, an empirical or fractal description of the drainage process combined with the Burdine [1953] or Mualem [1976] integral equations to develop a relative permeability function that shares parameters with the water retention function [e.g. Brooks and Corey, 1964; Van Genuchten, 1980; Tyler and Wheatcraft, 1990; Fuentes et al, 1996; Xu and Dong, 2004]. Sharing parameters between the water retention and relative permeability functions allows the prediction of one function if the other is known, but only through the use - and assumptions that go along with - the Burdine and Mualem models. Oversimplified representation of pore space geometry as a bundle of capillary tubes may result in discrepancies when comparing predictions from these models with the results of experimental data [Fischer and Celia, 1999; Tuller and Or, 2002].

Pore-network modeling is an alternative approach to predict relative permeability from measured water retention data [Fischer and Celia, 1999; Vogel and Roth, 2001; Metzger et al., 2007]; it involves optimization of bond- and site-size distributions in artificially generated lattices. However, non-unique solutions are easily obtained since various configurations of the pore-size distribution and interconnectivity can match those predicted by the measured water retention data [Vogel and Roth, 2001].
Fractals are iterative geometrical models for describing irregular and fragmented systems. Fractal geometry has been widely used to derive physically-based expressions for soil hydraulic functions (e.g., Giménez et al., 1997; Bird et al., 2000; Wang et al., 2005). Most fractal models, however, do not include an explicit description of incomplete pore connectivity, which can result in partial drainage of pores as the suction is increased. Thus, estimates of physically-based parameters - such as the mass fractal dimension - obtained by fitting these models to experimental water retention data may not be accurate. Because of incomplete drainage the resulting parameters might better be described as apparent values.

During drainage of a random porous medium, both the pore size distribution and the connectivity of pores determine the drained pore volume as function of suction. Cihan et al. [2007] presented a probabilistic-fractal approach to describe the drained pore space that explicitly incorporates the effect of connectivity among pores with different sizes and allows continuing drainage of pores at different suctions. In this study, we present a discrete version of their water retention model and use it to derive a new expression for the relative permeability function. This approach allows the relative permeability to be predicted directly from measured water retention data; no model fitting or parameters are required. We tested the performance of the new relative permeability expression using soil hydraulic data from the UNSODA database [Leij et al., 1996] and other highly regarded datasets collected from the literature.
2. Theory

2.1. Water Retention Function

Cihan et al. [2007] introduced a framework to quantitatively describe incomplete drainage and water retention function during drying of a random fractal porous medium. Their conceptual model assumes that as drying occurs, not all pores with a given size drain at the appropriate suction due to incomplete pore connectivity. The numbers of solids, $N_s$, of length $r$ in a mass prefractal porous medium is given by

$$N_s(r) = (b^i)^D$$

(1)

where $i$ is the iteration level, $b$ is the scale factor defined as the ratio of solid sizes at two successive iteration levels ($r_i/r_{i+1}$), and $D$ is the mass fractal dimension defined as 

$$D = \frac{\log N_s(r)}{\log r}$$

(2)

The numbers of pores, $N_p$, of length $r$ can be expressed as

$$N_p(r) = \left(b^E - b^D\right)b^{(i+1)D}$$

(2)

where $E$ is the Euclidean dimension. Depending upon the lacunarity of the prefractal porous medium, pores of length $r_0/b$ that did not drain at the appropriate suction, where $r_0$ is the characteristic length of the porous medium that shows fractal behavior, may remain full or drain into pores of length $r_0/b^2$, $r_0/b^3$, …, $r_0/b^i$ as $h \to \infty$. Cihan et al. [2007] proposed an approach to model this complex drainage process. Figure 3.1 shows a conceptual representation of their approach for a 2-D fractal porous medium with a unit length, $b=4$, $D=\log 10/\log 4=1.660…$ and $i=2$. An initially ($i=0$) saturated porous medium (Figure 3.1a) begins to drain by applying suction to the bottom. No flow occurs across the left and right sides, and all draining pores are assumed to retain a film of water. Six large pores with a length of $1/4$ are present. At the first iteration ($i=1$), five of the six
large pores that are connected from top to bottom, drain as shown with white color at Figure 3.1b. The non-draining large pore at the left side is connected with smaller pores of length of 1/16 and drains at iteration level 2. Nine of the sixty 1/16 sized pores are disconnected and remain water-filled at the end of drainage (Figure 3.1c).

Generalization of the above procedures to a porous medium with arbitrary fractal dimension and scale factor can be accomplished as follows. At iteration level 1, which corresponds to the air entry value or minimum capillary pressure, a \( P_1 \) fraction of the \( r_1 \) (=\( r_0/b \)) pores drain. This drained fraction can be expressed as \( P_1 N_p^{(1)}/b^3 \), where \( N_p^{(1)}/b^3 \) is the proportion of the largest pores within the whole volume. At iteration level 2, a \( P_2 \) fraction of the \( r_2 \) (=\( r_0/b^2 \)) pores and the remaining water volume in \( r_1 \) pores from iteration level 1 drain. The total fraction of draining water volume at \( i=2 \) can be expressed by \\
\[ P_2 \left[ N_p^{(2)}/b^6 + (1-P_1) N_p^{(1)}/b^3 \right]. \]

Cumulatively, after two iterations the volumetric fraction of water remaining in \( r_0/b \)- and \( r_0/b^2 \)-sized pores is given by

\[
\frac{N_p^{(2)}}{b^6} + (1-P_1) \frac{N_p^{(1)}}{b^3} - P_2 \left[ \frac{N_p^{(2)}}{b^6} + (1-P_1) \frac{N_p^{(1)}}{b^3} \right] = (1-P_2) \frac{N_p^{(2)}}{b^6} + (1-P_2) (1-P_1) \frac{N_p^{(1)}}{b^3}
\]

The proportion of water draining from the connected pores between any two successive iteration levels can be generalized as,
\[ i = 1 \quad \theta_0 - \theta_i = P_1 \frac{N_p^{(i)}}{b^{E}} \]

\[ i = 2 \quad \theta_1 - \theta_2 = P_2 \left[ \frac{N_p^{(2)}}{b^{2E}} + \left(1 - P_1\right) \frac{N_p^{(1)}}{b^{E}} \right] \]

\[ i = 3 \quad \theta_2 - \theta_3 = P_3 \left[ \frac{N_p^{(3)}}{b^{3E}} + \left(1 - P_2\right) \frac{N_p^{(2)}}{b^{2E}} + \left(1 - P_1\right) \frac{N_p^{(1)}}{b^{E}} \right] \]

\[ \vdots \]

\[ i = j \quad \theta_{j-1} - \theta_j = P_j \left[ \frac{N_p^{(j)}}{b^{jE}} + \left(1 - P_{j-1}\right) \frac{N_p^{(j-1)}}{b^{(j-1)E}} + \cdots + \left(1 - P_1\right) \frac{N_p^{(1)}}{b^{E}} \right] \]

where \( \theta_1, \theta_2, \theta_3, \ldots \) are the volumetric water contents corresponding to the suction levels \( n = 1, 2, 3, \ldots \), \( \theta_0 \) is the saturated water content, and \( P_i \) is the probability of drainage of the remaining pore volume at any \( i \) or any corresponding suction. Summation of all terms in (3) gives the total drained water content, \( \theta_d \) at any \( i \) or any corresponding capillary pressure, which is expressed in symbolic form as

\[ \theta_d(j) = \sum_{i=1}^{j} \sum_{m=i}^{j} \frac{N_p^{(i)}}{b^{mE}} P_m \prod_{k=i}^{m-1} (1 - P_k) \]

(4)

Then, if the water content is defined by

\[ \theta = \theta_0 - \theta_d(j) \]

(5)

\( \theta \) can be expressed as

\[ \theta = \sum_{i=1}^{j} \frac{N_p^{(i)}}{b^{iE}} \prod_{k=i}^{j} (1 - P_k) + \sum_{i=j+1}^{n} \frac{N_p^{(i)}}{b^{iE}} \]

(6)

\[ = \sum_{i=1}^{j} \frac{N_p^{(i)}}{b^{iE}} \exp \left\{ \sum_{k=i}^{j} \ln[(1 - P_k)] \right\} + \sum_{i=j+1}^{n} \frac{N_p^{(i)}}{b^{iE}} \]
Invoking the Young-Laplace expression [de Gennes et al., 2004], $1/b^i$ in equation (6) can be replaced with the normalized capillary pressure, $h_{\text{min}}/h$. The $P_i$ values contain information about the connectivity of the pore system and are independent of any assumed fractal drainage behavior. $P_i$ can be expressed as [Cihan et al., 2007]:

$$P_i = \frac{\theta_{r-i} - \theta_j}{\sum_{n=1}^{i} \frac{N_p^{(n)}}{b^{nE} \prod_{k=n}^{i-1} (1 - P_k)}}$$

(7)

and $P_1, P_2, \ldots, P_i$ values can be estimated inversely from the water retention curve if $b, D$, and $i$ values are known a priori for a fractal porous medium.

2.2. Relative Permeability: Probabilistic Capillary-Connectivity (PCC) Model

Neglecting inertial effects, the mean velocity of a fluid, $u$, in a narrow tube of radius, $r_t$, is given by Poiseuille’s equation, i.e.

$$u = -\frac{Cr_t^2 \rho g \frac{dh}{dl}}{\mu}$$

(8)

where $C$ is a shape factor, $\mu$ is the dynamic viscosity, $\rho$ is the density, $g$ is the gravitational acceleration, and $dh/dl$ is the potential gradient driving the fluid flow in the tube. If the porous medium is considered to be made up of channels of different sizes, Poiseuille’s equation approaches Darcy’s law, which expresses the mean velocity of a fluid in a porous medium and can be written as

$$q = -\frac{k \rho g \frac{dh}{dl}}{\mu}$$

(9)

where $k$ is equivalent to $\langle Cr_t^2 \rangle$, an averaged quantity for porous media. The shape factor $C$, changes depending on the geometry of the pore.
Cihan et al. [2008] proposed a fractal-based method, the “Probabilistic Capillary-Connectivity Model” (PCC), to describe the permeability of saturated porous media. Their method separates the system into multiple connected flow paths or networks. We employ this same methodology to formulate the relative permeability function. Consider an initially saturated network consisting of only the largest pores of size $r_0/b$ connected from one end to the other in the direction of flow. Following Poiseuille’s equation, the mean velocity of water following such a pathway is proportional to $r_0^2/b^2$. At iteration level 1 of the drainage, the permeability decreases as the connected largest pores sized $r_0/b$ are draining. The probability for the existence of such a draining pathway is equal to the proportion of the largest connected pores in the system (i.e. $P_1 N_p^{(1)} / b^3$). The remaining proportion of water in pores of size $r_0/b$ is given by $(1-P_1) N_p^{(1)} / b^3$; these pores may be completely unconnected or connected with smaller pores of size $r_0/b^2$ to form a different flow pathway. There might also be a network formed by only the $r_0/b^2$-sized pores. The probability for the existence of a network containing $r_0/b^2$-sized pores or $r_0/b$- and $r_0/b^2$-sized pores is written as $P_2 (N_p^{(2)} / b^{2+3} + (1-P_1) N_p^{(1)} / b^3 )$, where $P_2$, as defined before, represents the connected proportion of water-filled pores in networks formed by $r_0/b^2$- or larger-sized pores, which will drain at iteration level 2. Since flow is controlled by the smallest pores within a network of different-sized connected water-filled pores, the mean velocity of water following a pathway consisting of $r_0/b$- and $r_0/b^2$-sized pores is assumed to be proportional to cross sectional area of the smaller pores, i.e. $r_0/b^2$. In generalized form, the pore areas controlling flow in the different flow paths, multiplied by their associated probabilities, are written as:
\[ i = 1 \quad P_i \frac{N_p^{(i)} r_0^2}{b_i^{2E} b^2} \]

\[ i = 2 \quad P_2 \left[ \frac{N_p^{(2)} r_0^2}{b_2^{2E}} + \left( 1 - P_1 \right) \frac{N_p^{(1)} r_0^2}{b_1^{2E}} \right] \]

\[ i = 3 \quad P_3 \left[ \frac{N_p^{(3)} r_0^2}{b_3^{2E}} + \left( 1 - P_2 \right) \frac{N_p^{(2)} r_0^2}{b_2^{2E}} + \left( 1 - P_1 \right) \frac{N_p^{(1)} r_0^2}{b_1^{2E}} \right] \]

\[ \vdots \quad \vdots \]

\[ i = n \quad P_n \left[ \frac{N_p^{(n)} r_0^2}{b_n^{2E}} \right] \]

\[ k = C r_0^2 \sum_{i=1}^{n} \sum_{j=i}^{n} \frac{N_p^{(i)} P_j}{b_i^{2E} b_j^{2E}} \prod_{k=i}^{j-1} \left( 1 - P_k \right) \quad \text{(11)} \]

where \( n \) is the last iteration level of the fractal porous medium, and the pore shape factor \( C \) is assumed to be constant for all pores.

Assuming that drainage develops from the largest pores to the smallest pores sequentially, permeability of draining porous medium can be expressed as

\[ k_w (m) = k - C r_0^2 \sum_{i=1}^{m} \sum_{j=i}^{m} \frac{N_p^{(i)} P_j}{b_i^{2E} b_j^{2E}} \prod_{k=i}^{j-1} \left( 1 - P_k \right) \quad \text{(12)} \]

where \( 1 \leq m \leq n \) is the \( m \)-th drainage iteration level or suction level. Comparing equation (10) with equation(3), equation (12) can be expressed as

\[ k_w (m) = k - C \sum_{i=1}^{m} \Delta \theta \frac{r_0^2}{b_i^{2E}} \quad \text{(13)} \]

Since relative permeability is defined by \( k_{rw} = k_w / k \), i.e.
When \( m \) is equal to \( n \), \( k_{rw} \) is 1. By applying the Young-Laplace expression [de Gennes et al., 2004], equation (14) can be expressed in terms of the suction \( h \), giving:

\[
k_{rw}(m) = 1 - \frac{\sum_{i=1}^{m} \Delta \theta_i / b_i^2}{\sum_{i=1}^{n} \Delta \theta_i / b_i^2}
\]

Equation (15) allows the prediction of the relative permeability by direct use of the measured points from a water retention curve without the need for fitting. Due to the discrete nature of the PCC model, when the water retention data is known, the discrete-PCC relative permeability function can be incorporated into numerical algorithms to solve unsaturated flow equation. However, some sort of interpolation among calculated \( k_{rw} \) values may be needed to find its unknown values at varying suctions.

If a system is assumed to consist of continuously distributed pores, equation (15) can be converted to the continuous case as:

\[
k_w = k - C \sum_{i=1}^{n} \left( \frac{\Delta \theta_i}{\Delta r_i} \right) r_i^2 \Delta r_i
\]

\[
\approx k - C \lim_{\Delta r_1, \Delta r_2, \Delta r_3 \to 0} \left\{ \frac{\Delta \theta_1}{\Delta r_1} r_1^2 \Delta r_1 + \frac{\Delta \theta_2}{\Delta r_2} r_2^2 \Delta r_2 + \frac{\Delta \theta_3}{\Delta r_3} r_3^2 \Delta r_3 + \cdots \right\} = k - C \int r \theta'(r) r^2 dr
\]

and the relative permeability is expressed as

\[
k_{rw} = 1 - \frac{\int_{1}^{r} \theta'(r^*) r^* 2 dr^*}{\int_{h_{min}}^{h_{max}} \theta'(r^*) r^* 2 dr^*} = \frac{r_{max}}{h_{max}} \frac{h_{min}}{h}
\]
where $r_{\text{max}}$ is the largest pore size, and $h_{\text{max}}$ is the highest capillary pressure to drain the largest pores under the effect of capillary forces. Equation (17) is derived by assuming continuous pore size distribution and is similar in form to the Burdine [1953] equation.

In this study, we will concentrate on evaluating the discrete function given by equation (15), since its application does not require a fitting procedure, and unlike equation (17), it does not require a priori knowledge of the minimum suction ($h_{\text{min}}$). We will test equation (15) against the UNSODA database [Leij et al., 1996] and other previously published soil hydraulic measurements of water retention and relative permeability.

3. Data Sets and Model Testing

UNSODA is one of the largest soil data sets that includes suction-water content-relative permeability data for a wide range of soils from clay to gravel. Within UNSODA, only 35 data sets are paired: i.e., the water content and relative permeability measurements were collected at the same capillary pressures. We restricted our comparison to the paired data because we have not, as of yet, established a means to estimate the relative permeability at suctions in between those included in the actual measurements. Another five paired data sets were located in the literature for more detailed analysis. These data sets were for the following materials: Yolo light clay [Moore, 1934], Guelph loam [Elrick and Bowman, 1964], superstition sand [Richards, 1952], Hygiene sandstone [Brooks and Corey, 1964], and Berea sandstone [Brooks and Corey, 1964]. The Yolo light clay and Guelph loam data sets also appear in the UNSODA database. These five data sets are well documented and have been extensively investigated [Van Genuchten, 1980; Fredlund et al., 1994].
Predictions of equation (15) were compared with the popular empirical Van Genuchten-Mualem (VG-M) [1980] relative permeability function. The VG water retention, and VG-M relative permeability, are expressed as function of suction in the following equations,

\[ S = S_r + (1 - S_r) \left[ 1 + (\alpha h)^n \right]^{-m}; \quad m = 1 - 1/n \]  

\[ k_{rw}(h) = \frac{\left\{ 1 - (\alpha h)^{n-1} \left[ 1 + (\alpha h)^n \right]^{-m} \right\}^2}{\left[ 1 + (\alpha h)^n \right]^{m/2}}; \quad m = 1 - 1/n \]  

where \( S \) is the saturation, and \( S_r \) is the residual saturation. The VG-M model parameters \((\alpha, n, \text{ and } S_r)\) were obtained by fitting to the measured water retention data sets using non-linear regression (Marquardt method) in SAS [SAS Institute, 1999]. All of the fits converged according to the SAS default convergence criterion [SAS Institute, 1999]. The average coefficient of determination \((R^2)\) between the measured and predicted saturations for equation (18) fitted to the 40 water retention data sets was 0.999.

The accuracy of the predictions of relative permeability by the two models was evaluated by the root mean square error (RMSE). We also computed the log-RMSE (LRMSE) based on the logarithms of the measured and predicted \(k_{rw}\) values to quantify the performance of both models at low relative permeabilities. Paired t-tests were used to evaluate if the differences in RMSE and LRMSE values between the two models were statistically significant at \( p < 0.05 \) (5% level of significance).
4. Results

Figure 3.2 shows the differences in the performance of the discrete-PCC (red circles) and the VG-M (blue squares) models for the pooled forty data sets. A 1:1 line shows the optimal performance and the discrete-PCC predictions were generally closer. The mean RMSE for the predicted $k_{rw}$ from equation (15) was 0.128, while for the predicted $k_{rw}$ from the VG-M model, the mean RMSE was 0.140. The mean LRMSE for the discrete-PCC model was 0.813, while for the VG-M model it was 1.555. Paired t-tests for the 40 data sets showed that mean RMSEs of the two models were not significantly different, while the mean LRMSEs were significantly different at $p < 0.05$. These results indicate that overall the discrete-PCC method (15) predicted the measured data better than the VG-M (19) at $p < 0.05$.

We also present individual comparisons for the five soils collected from the literature (Figures 3.3-7). We should note that only the five soils shown in Figures 3.3-7 were found; no selective screening was done to eliminate data sets that produced less than ideal results. Table 3.1 presents the estimated parameters of the VG function fitted to the water retention data. For the discrete-PCC model, the RMSEs calculated ranged between 0.039 and 0.148 with a mean RMSE of 0.090 and the LRMSEs ranged between 0.227 and 0.489 with a mean LRMSE of 0.401. The RMSEs from the VG-M model ranged between 0.113 and 0.271 with an average of 0.179 and the LRMSE values ranged between 0.820 and 2.173 with a mean LRMSE of 1.501(Figures 3.3-7). The direct PCC prediction resulted in smaller RMSE and LRMSE values for each case. Generally, the VG-M model under predicted the relative permeabilities. Paired t-test showed that mean
RMSE and LRMSE values of the new method predictions were significantly less at $p < 0.05$ than those of the VG-M for these five soils.

4. Discussion and Conclusions

We combined the probability of drainage concept and the PCC approach introduced by Cihan et al. [2007] and [2008], respectively, to derive the relative permeability function for drainage of random mass fractal porous media, i.e., the discrete-PCC model. The discrete-PCC model allows estimation of the relative permeability directly from measured water retention data and does not require any curve fitting.

The performance of the discrete-PCC was tested on forty data sets and compared with the VG-M model. Results indicate that overall, the discrete-PCC method (equation 15) predicted the relative permeability significantly better than the VG-M. It should be noted that some data sets within UNSODA database appear to be questionable. For instance, the relative permeability of some clay soils decreased rapidly with a small increase in suction. This might indicate the presence of macropores or fractures resulting in considerable momentum losses thereby flawing the assumptions behind Darcy’s law and capillary equilibrium based on the Young-Laplace equation. In these cases both models resulted in inadequate predictions of relative permeability.

We also analyzed individual predictions of the models for five soils used by many researchers in previous publications on this subject. The VG-M model generally under predicted the measured data for all of the five soils. In contrast, the discrete-PCC model predicted the measured data reasonably well except that its predicted values showed relatively greater differences from the measured data at high suctions for the Berea and Hygiene sandstones (see Figures 3.6 and 3.7).
The discrete-PCC relative permeability function can be used within numerical algorithms to solve the partial differential equations governing unsaturated flow. Some sort of interpolation scheme may be needed to compute $k_{rw}$ for suctions not included in the experimental water retention dataset. The present model is restricted to monotonic drainage from saturation. However, there is no theoretical reason why it cannot be adapted to wetting up and thereby extended to incorporate hysteresis. However, few relative permeability data are available for model testing in the wetting case.
LIST OF REFERENCES
References


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Cihan A., M. Sukop, J. S. Tyner, E. Perfect, and H. Huang (2008), Analytical predictions and lattice Boltzmann simulations of intrinsic permeability for mass fractal porous media, submitted to *Vadose Zone J.*


Table 3.1. Model parameters ($\alpha$, $n$, and $S_r$) of VG-water retention function fitted to measured water retention for published paired-data sets.

<table>
<thead>
<tr>
<th>Soils</th>
<th>Residual saturation, $S_r$</th>
<th>$\alpha$ (cm$^{-1}$)</th>
<th>$n$</th>
<th>$R^2$ (water retention)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Yolo light clay [Moore, 1934]</td>
<td>0.430</td>
<td>0.025</td>
<td>1.776</td>
<td>0.998</td>
</tr>
<tr>
<td>Guelph loam [Elrick and Bowman, 1964]</td>
<td>0.414</td>
<td>0.013</td>
<td>1.946</td>
<td>0.994</td>
</tr>
<tr>
<td>Superstition sand [Richards, 1952]</td>
<td>0.287</td>
<td>0.028</td>
<td>5.100</td>
<td>0.999</td>
</tr>
<tr>
<td>Berea sandstone [Brooks and Corey, 1964]</td>
<td>0.328</td>
<td>0.019</td>
<td>8.928</td>
<td>0.996</td>
</tr>
<tr>
<td>Hygiene sandstone [Brooks and Corey, 1964]</td>
<td>0.615</td>
<td>0.016</td>
<td>10.64</td>
<td>0.995</td>
</tr>
</tbody>
</table>
Figure 3.1. Idealized example realization of a drying random 2-d fractal porous medium with $b = 4$, the last iteration level $i = 2$ and $D = 1.660…$ (Black = solid, white = air-filled pore, and blue = water-filled pore).
Figure 3.2. Comparison of the relative permeability predictions from direct-PCC and the VG-M with the measured relative permeabilities from the entire forty data sets.
Figure 3.3. Comparison of measured and predicted relative permeability curves of the Yolo light clay.
Figure 3.4. Comparison of measured relative permeability and the predicted relative permeability curves of the Guelph loam.
Figure 3.5. Comparison of measured relative permeability and predicted relative permeability curves of the Superstition sand.
Figure 3.6. Comparison of measured relative permeability and predicted relative permeability curves of the Berea sandstone.
Figure 3.7. Comparison of measured relative permeability and predicted relative permeability curves of the Hygiene sandstone.
PART IV
ANALYTICAL SOLUTION FOR SOLUTE TRANSPORT THROUGH
A MACROPOROUS MEDIUM: EFFECT OF
BOUNDARY CONDITIONS
Abstract

This study presents analytical solutions of the advective solute transport in a macropore with simultaneous diffusion into an unbounded soil matrix. We obtained three set of solutions including cases of: 1) an instantaneous release of solutes, 2) a pulse type release of solute, and 3) a constant concentration of solute at the top of a macropore. A system of two governing equations was solved by the Laplace Transform method for solute concentration as a function of space and time. Substituting the useful asymptotic approximations of the modified Bessel functions, we obtained the approximate solutions for the all three cases. Comparisons between the exact and approximate solutions show that the asymptotic approximations result in very accurate results for short times of solute movement.

1. Introduction

Many researchers have analytical solutions of the advection-dispersion transport equation (ADE) to describe the movement of adsorbing or non-adsorbing solutes into a soil matrix from a fracture or macropore. However, computing such solutions in cylindrical coordinates can be difficult compared to similar solutions in rectangular coordinates.

Van Genuchten et al. [1984] obtained closed form analytical solutions of solute migration from a constant concentration source in a cylindrical macropore with radial matrix diffusion. Van Genuchten et al. [1984] also presented approximate solutions using asymptotic expansions of the modified Bessel functions, while neglecting dispersion. Their approximate solutions proved to be valid for short times.
Macropore-matrix system approach was also used for the investigation of sorbing and nonsorbing solutes. *Young and Ball* [1998] used a column in which the center was filled with sand and the annulus forming the matrix was filled with a low permeability material (deltaic soil). Pore diffusion coefficients in the matrix were estimated by fitting to a numerical solution of the 2-D ADE for a time dependent injection of solutes from the top of the column. The model equation included the advective-dispersive transport of the solutes in the central sandy part and only diffusion in the in matrix. Recently, *Rahman et al.* [2004] studied the sorption kinetics of organic contaminants migrating with a pulse type injection from a cylindrical macropore to the soil matrix using a similar experimental setup given in *Young and Ball* [1998]. Neglecting the cylindrical shape of the macropore in their system, *Rahman et al.* [2004] applied the analytical solution given by *Grisak and Pickens* [1981] with some errors associated in their prediction of sorption parameters.

*Allaire et al.* [2002] conducted numerical and experimental studies for the effect of initial and boundary conditions applied to a macropore-matrix system. They obtained numerical solutions in Cartesian coordinates by applying constant and pulse type injections for a system of macropores with regular or irregular geometries. They concluded that for the prediction of the breakthrough curves, highly tortuous discrete macropores in water and solute transport models could be simplified as straight macropores.

This study attempts to fill a missing portion of the literature: analytical solutions of solute transport within a macropore-matrix system having cylindrical coordinates. We obtain analytical solutions for solute transport in a macropore with radial diffusion into a
surrounding soil matrix. Three types of solutions are presented including: 1) an instantaneous release of solutes, 2) a pulse type release, and 3) a constant concentration source at the top of macropore. Like Grisak and Pickens [1981] and Rahman et al. [2004], we assume that solute transport within the macropore is governed by vertical advection only, while solute transport within the matrix is governed by radial diffusion only.

2. Governing Equations and Exact Solutions

In the presence of diffusion from a cylindrical macropore into a surrounding soil matrix (Figure 4.1), averaging the ADE over the cross section of the macropore gives the advective transport equation for a contaminant migrating with a mean velocity of water in the macropore [Rahman et al., 2004; Van Genuchten et al., 1984]. The system of equations for macropore and matrix regions are given by

\[
R_m \frac{\partial C_m}{\partial t} = -v_m \frac{\partial C_m}{\partial z} + \frac{2}{r_m \theta_m} \frac{D_a \partial C_a}{\partial r} \bigg|_{r=r_m} \tag{1}
\]

\[
R_a \frac{\partial C_a}{\partial t} = \frac{D_a}{r} \frac{\partial}{\partial r} \left( r \frac{\partial C_a}{\partial r} \right) \tag{2}
\]

The first equation defines the average solute concentration in the macropore, while the second one defines the solute migration in the matrix, where \( C \) (\( M L^{-3} \)) is solute concentration \( R \) (dimensionless) is retardation factor, \( \theta (L^3 L^{-3}) \) is the volumetric water content, \( D \) is the diffusion coefficient (\( L^2 T^{-1} \)), \( r_m \) is the macropore radius, \( r \) is the radial distance from the center of the macropore (\( L \)), \( t \) is elapsed time (\( T \)), \( v \) is the mean velocity (\( L T^{-1} \)), \( z \) is the vertical distance (\( L \)), and the subscripts \( m \) and \( a \) denote the macropore and the matrix, respectively (Figure 4.1).
2.1. Case 1: Instantaneous Release of Solutes

The initial and boundary conditions for an instantaneous release of solutes are given as

\[
\begin{align*}
C_m(z,0) &= \frac{M}{A_m} \delta(z - z_0) ; \quad 0 < z_0 \leq z < \infty, 0 \leq r \leq r_m, \\
C_m(0,t) &= 0 \\
C_a(r,z,0) &= 0 \\
\frac{\partial C_a}{\partial r}(\infty,z,t) &= 0, C_a(r_m,z,t) = C_m(z,t) ; \quad r_m \leq r < \infty
\end{align*}
\]

(3)

where \( M \) is the mass of the contaminants released instantaneously into the area of the macropore \( (A_m) \), \( \delta(z - z_0) \) is the Dirac Delta function, and \( z_0 \) is the vertical distance from the origin where the solute is released. Taking the Laplace transform of the system above, we obtain

\[
\frac{d\bar{C}_m}{dz} + \frac{R_m s}{v_m} \bar{C}_m = \frac{2}{r_m \theta_m v_m} \frac{\partial \bar{C}_a}{\partial r} \bigg|_{r=r_m} + \frac{M}{A_m v_m} \delta(z - z_0)
\]

(4)

\[
\frac{d^2 \bar{C}_a}{dr^2} + \frac{1}{r} \frac{d \bar{C}_a}{dr} - \frac{R_a s}{D_a} \bar{C}_a = 0
\]

(5)

where

\[
\bar{C}_m = \int_0^\infty C_m(-st) \, dt, \quad \bar{C}_a = \int_0^\infty C_a(-st) \, dt
\]

(6)

Likewise, the boundary conditions are transformed

\[
\bar{C}_m(0,s) = 0 \\
\bar{C}_a(r_m,z,s) = \bar{C}_m(z,s) ; \quad \frac{\partial \bar{C}_a}{\partial r}(\infty,z,s) = 0
\]

(7)

where \( s \) is the Laplace transform parameter. Solving the system in (4)-(5) subject to the boundary conditions (7), we find
\[
\tilde{C}_m(z,s) = \frac{M R_m}{A_m v_m} \exp\left\{- \frac{R_m (z-z_0)}{v_m} \left[ s + \frac{2 \theta_m \sqrt{D_a R_a}}{r_m \theta_m R_m} \sqrt{s} \frac{K_1 \left( r_m \sqrt{R_a s/D_a} \right)}{K_0 \left( r_m \sqrt{R_a s/D_a} \right)} \right] \right\}
\]

(8)

\[
\bar{C}_m(z,r,s) = \frac{\tilde{C}_m(z,s)}{K_0 \left( r_m \sqrt{R_a s/D_a} \right)}
\]

(9)

where \(K_0(\cdot)\) and \(K_1(\cdot)\) are the modified Bessel functions of the second kind of orders zero and one, respectively. Laplace inversion for equations (8) and (9) are defined by

\[
C_m = \frac{1}{2\pi i} \int_{s=y-i\infty}^{s=y+i\infty} \tilde{C}_m \exp(st) ds, \quad C_a = \frac{1}{2\pi i} \int_{s=y-i\infty}^{s=y+i\infty} \bar{C}_a \exp(st) ds
\]

(10)

Equations (10) have a branch point at the origin where they are multi-valued and do not have isolated poles in the \(s\) plane. In this case, the general contour integration formula is given by [Ozisik, 1980]

\[
C(t) = \frac{1}{2\pi i} \int_{\gamma} \exp(-xt) \left[ \tilde{C} \bigg|_{z=x+\exp(-i\pi)} - \tilde{C} \bigg|_{z=x+\exp(i\pi)} \right] dx + \lim_{\rho \to 0} \frac{1}{2\pi} \int_{-\pi}^{\pi} \exp\left[ \rho \exp(i\alpha) \right] \tilde{C} \bigg|_{z=x+\rho \exp(i\alpha)} \rho \exp(i\alpha) d\alpha
\]

(11)

where \(\tilde{C}\) is the transformed function. After substituting equation (8) into (11), we obtain

\[
C_m(z,t) = \frac{M R_m}{2\pi A_m v_m} \exp\left\{ \frac{(z-z_0) R_m}{v_m} - t \right\} \left\{ \exp\left[ - \frac{2 \theta_m \sqrt{D_a R_a (z-z_0)} \sqrt{x} \exp(-i \pi/2)}{r_m \theta_m v_m} \frac{K_1 \left( r_m \sqrt{R_a x/D_a} \right)}{K_0 \left( r_m \sqrt{R_a x/D_a} \right)} \right] - \exp\left[ - \frac{2 \theta_m \sqrt{D_a R_a (z-z_0)} \sqrt{x} \exp(i \pi/2)}{r_m \theta_m v_m} \frac{K_1 \left( r_m \sqrt{R_a x/D_a} \right)}{K_0 \left( r_m \sqrt{R_a x/D_a} \right)} \right] \right\} dx
\]

(12)
where \( \exp(\pm \pi i) = 1 \), \( \exp(\pm \pi i / 2) = \pm i \), and the second integral in equation (11) becomes zero. Substituting variables \( \mu^2 = x R / D_a \) and by using the following relationship [Debnath, 1995]

\[
K_v\left[y \exp\left(\mp \pi i / 2\right)\right] = \pm \frac{1}{2} \pi i \exp\left(\mp \pi i / 2\right)\left[-J_v(y) \pm i Y_v(y)\right]
\]

where \( J_v() \) and \( Y_v() \) are the Bessel functions of the first and second kinds of order \( v \), and \( K_v() \) is the modified Bessel Function of the second kind of order \( v \), equation (12) reduces to

\[
C_m(z,t) = \frac{D M R_m}{\pi A r_m R_a} \int_0^{\infty} \mu \exp\left\{ \left(\frac{z-z_0}{R_m} - t\right) \frac{D_a}{R_a} \mu^2 \right\} \frac{1}{i} \exp\left[ -2 \theta_a D_a \frac{(z-z_0) \mu}{r_m \theta_m} \left( J_1(r_m \mu) + i Y_1(r_m \mu) \right) + J_0(r_m \mu) + i Y_0(r_m \mu) \right] d\mu
\]

(14)

Multiplying the terms in the exponentials of (14) by the conjugates \( J_0(r_m \mu) \pm i Y_0(r_m \mu) \) eliminates the complex numbers from the integral, and the solution can be simplified as

\[
C_m(z,t) = \frac{2 D M R_m}{\pi A r_m R_a} \int_0^{\infty} \mu \sin\left(\frac{z-z_0}{R_m} - t\right) \frac{D_a}{R_a} \mu^2 \frac{2 \theta_a D_a (z-z_0) \mu}{r_m \theta_m} \left( \frac{J_1(r_m \mu) Y_1(r_m \mu) - Y_0(r_m \mu) J_1(r_m \mu)}{J_0(r_m \mu)^2 + Y_0(r_m \mu)^2} \right) d\mu
\]

(15)

Likewise, we can also evaluate \( C_a(r,z,t) \) as follows.
After substituting equation (13) into (16) and multiplying the complex terms by their conjugates \( J_0(r_m \mu) \pm i Y_0(r_m \mu) \), we obtain

\[
C_a(r, z, t) = \frac{2 D_a M R_m}{\pi A_m} \int_0^1 \frac{\mu \exp \left[ \frac{(z - z_0) R_m - t}{R_m} \right] D_a R_m^2}{i} \exp \left[ \frac{(z - z_0) \mu}{R_m} \right] K_0 \left[ r_m \mu \exp(-i \pi/2) \right] - \exp \left[ -i \frac{2 \theta_a D_a (z - z_0) \mu}{r_m \theta_m v_m} \exp \left[ i \pi/2 \right] K_0 \left[ r_m \exp(i \pi/2) \right] \right] \] (16)

\[
\sin \left[ -i \frac{2 \theta_a D_a (z - z_0) \mu}{r_m \theta_m v_m} \left( J_0(r_m \mu) Y_1(r_m \mu) - J_1(r_m \mu) Y_0(r_m \mu) \right) \right] + \cos \left[ -i \frac{2 \theta_a D_a (z - z_0) \mu}{r_m \theta_m v_m} \left( J_0(r_m \mu) Y_1(r_m \mu) - J_1(r_m \mu) Y_0(r_m \mu) \right) \right]
\]

\[
\left[ J_0(r_m \mu) Y_0(r_m \mu) - Y_0(r_m \mu) J_0(r_m \mu) \right] d \mu
\]

It can be seen that equation (17) is identical to equation (15) when \( r = r_m \). The numerical integrations of equations (15) and (18) can be made using software such as Mathcad® or Mathematica®. When computing the solutions at very small times, the following approximations [VanGenuchten et al., 1984]

\[
\frac{K_1 \left( r_m \sqrt{R_a s / D_a} \right)}{K_0 \left( r_m \sqrt{R_a s / D_a} \right)} \approx 1 + \frac{1}{2 r_m \sqrt{R_a s / D_a}}; \quad \frac{K_0 \left( r \sqrt{R_a s / D_a} \right)}{K_0 \left( r_m \sqrt{R_a s / D_a} \right)} \approx \sqrt{\frac{r_m}{r \sqrt{R_a s / D_a}}} \quad (18)
\]
can be substituted into (8) and (9) to obtain the approximate analytical solutions

\[
C_m(z,t) = \frac{M R_m \theta_a \sqrt{D_a R_a} (z - z_0)}{\sqrt{\pi} r_m A_m v_m^2 \theta_m \left[t - R_m (z - z_0)/v_m\right]^{3/2}} \cdot 
\exp \left\{ - \frac{D_a \theta_a (z - z_0)}{r_m^2 \theta_m R_m v_m} \left[1 + \frac{\theta_a R_a (z - z_0)}{\theta_m v_m \left[t - R_m (z - z_0)/v_m\right]}\right] \right\}
\]

(19)

\[
C_a(r,z,t) = \frac{M R_m \sqrt{R_a}}{\sqrt{\pi} A_m v_m \left[t - R_m (z - z_0)/v_m\right]^{3/2}} \sqrt{\frac{r_m}{r}} \left[\frac{\theta_a \sqrt{D_a} (z - z_0)}{r_m \theta_m v_m} + \frac{(r - r_m)}{2D_a}\right] 
\exp \left\{ - \frac{D_a \theta_a (z - z_0)}{r_m^2 \theta_m R_m v_m} \left[1 + \frac{\theta_a R_a (z - z_0)}{\theta_m v_m \left[t - R_m (z - z_0)/v_m\right]}\right] \right\} - 
\frac{R_a (r - r_m)}{\left[t - R_m (z - z_0)/v_m\right]} \left[\frac{\theta_a (z - z_0)}{r_m \theta_m v_m} + \frac{(r - r_m)}{4D_a}\right].
\]

(20)

2.2. Case 2: Constant Concentration Boundary Condition

The initial and boundary conditions for the fixed concentration source are given as

\[
C_m(z,0) = 0, \quad C_a(r,z,0) = 0
\]

\[
C_m(0,t) = C_0, \quad \frac{\partial C_a}{\partial r}(\varphi, z, t) = 0, C_a(r_m, z, t) = C_m(z, t)
\]

(21)

Taking the Laplace transform of the system above, we obtain

\[
\frac{d\bar{C}_m}{dz} + \frac{R_m s}{v_m} \bar{C}_m = 2 \frac{\theta_a D_a}{r_m \theta_m v_m} \frac{\partial \bar{C}_a}{\partial r} \bigg|_{r=r_m}
\]

(22)

\[
\frac{d^2\bar{C}_a}{dr^2} + \frac{1}{r} \frac{d\bar{C}_a}{dr} - \frac{R_a s}{D_a} \bar{C}_a = 0
\]

(23)

Likewise, the boundary conditions are transformed
The solutions of the system in (23)-(24) subject to the boundary conditions (24) are given by

\[
\overline{C}_m (z, s) = \frac{C_0}{s} \exp \left\{ - \frac{R_m z}{v_m} \left[ s + \frac{2 \theta_a \sqrt{D_a R_a}}{r_m \theta_m R_m} \sqrt{s} \frac{K_1 \left( r_m \sqrt{s / D_a} \right)}{K_0 \left( r_m \sqrt{s / D_a} \right)} \right] \right\},
\]

(25)

\[
\overline{C}_a (r, z, s) = \overline{C}_m (z, s) \frac{K_0 \left( r \sqrt{s / D_a} \right)}{K_0 \left( r_m \sqrt{s / D_a} \right)}
\]

(26)

The Laplace inversion of equations (25) and (26) are obtained by use of (11) following the same procedures as in Case 1, but in this case the second integral on the left hand side of (11) becomes equal to 1. The general solution for the concentration distribution in the macropore is given by

\[
C_m (z, t) = C_0 - \frac{2 C_0}{\pi} \int_0^\infty \frac{1}{\mu} \sin \left\{ - \frac{2 \theta_a D_a z \mu}{r_m \theta_m v_m} \frac{J_0 (r_m \mu) Y_1 (r_m \mu) - Y_0 (r_m \mu) J_1 (r_m \mu)}{J_0 (r_m \mu)^2 + Y_0 (r_m \mu)^2} \right\} \sin \left( \frac{z R_m}{v_m} \frac{D_a \mu^2}{R_a} - \frac{2 \theta_a D_a z \mu}{r_m \theta_m v_m} \frac{J_0 (r_m \mu) J_1 (r_m \mu) + Y_0 (r_m \mu) Y_1 (r_m \mu)}{J_0 (r_m \mu)^2 + Y_0 (r_m \mu)^2} \right) d \mu
\]

(27)

Van Genuchten et al. [equation 92, 1984] gave a solution similar to equation (27) for the concentration distribution in macropore, however, both the form and the computation of the equation (27) are simpler. The general solution for the concentration distribution in the matrix is given by
\[ C_a(r,z,t) = C_0 - \frac{2C_0}{\pi} \int_0^\infty \frac{1}{\mu} \left[ J_0 \left( \frac{r_n \mu}{(r_n \mu)^2 + (r_m \mu)^2} \right) \right. \]

\[ \exp \left[ \left( \frac{zR_m}{v_m} - t \right) \frac{D_a}{R_a} \mu^2 - \frac{2\theta_a D_a z \mu}{r_m \mu} \left( \frac{J_0(r_m \mu)J_1(r_m \mu) + Y_0(r_m \mu)Y_1(r_m \mu)}{J_0(r_m \mu)^2 + Y_0(r_m \mu)^2} \right) \right] \]

\[ \left\{ [J_0(r_m \mu)J_0(r \mu) + Y_0(r_m \mu)Y_0(r \mu)] \right\} \]

\[ \sin \left[ -\frac{2\theta_a D_a z \mu}{r_m \mu} \left( \frac{J_0(r_m \mu)Y_1(r_m \mu) - J_1(r_m \mu)Y_0(r_m \mu)}{J_0(r_m \mu)^2 + Y_0(r_m \mu)^2} \right) \right] + \]

\[ \cos \left[ -\frac{2\theta_a D_a z \mu}{r_m \mu} \left( \frac{J_0(r_m \mu)Y_1(r_m \mu) - J_1(r_m \mu)Y_0(r_m \mu)}{J_0(r_m \mu)^2 + Y_0(r_m \mu)^2} \right) \right] \]

\[ [J_0(r_m \mu)Y_0(r \mu) - Y_0(r_m \mu)J_0(r \mu)] d\mu \]

As in Case 1, for very small times, the approximate solutions can be given as

\[ C_m(z,t) \approx C_0 \exp \left( -\frac{\theta_a D_a z}{r_m^2 \mu} \right) \text{erfc} \left[ \frac{\theta_a \sqrt{D_a R_a} z}{r_m \mu \sqrt{t} \sqrt{z R_m/v_m}} \right] \]

\[ C_a(r,z,t) \approx C_0 \sqrt{r_m} \exp \left( -\frac{\theta_a D_a z}{r_m^2 \mu} \right) \text{erfc} \left[ \frac{2\theta_a \sqrt{D_a R_a} z + (r - r_m) \sqrt{R_a}}{2r_m \mu \sqrt{t} \sqrt{z R_m/v_m}} \right] \]

which are the same as those given previously by Van Genuchten et al., [equations (95) and (104), 1984].

**2.3. Case 3: Pulse Type Boundary Condition**

The initial and boundary conditions for the pulse-type release of solutes are the same as given in Case 2 except that the boundary condition at \( z = 0 \) is replaced with

\[ C_m(0,t) = \begin{cases} 
C_0; & t \leq t_0 \\
0; & t > t_0
\end{cases} \]

\[ 104 \]
The Laplace transform of (31) gives $\bar{C}_m(0, s) = C_0 (1 - e^{-t_0}) / s$. The general solutions for this case have been obtained by following the same methods given in Case 1 and Case 2. The general solution for the concentration distribution in the macropore can be written in terms of the solutions in Case 2

$$C_m(z, t) = C_{m, 2}(z, t); \quad t \leq t_0$$

$$C_m(z, t) = C_{m, 2}(z, t) - C_{m, 2}(z, t - t_0); \quad t > t_0$$

where the sub indices 2 were used to denote the solution obtained in Case 2. Likewise, the solution for the matrix region is given as

$$C_a(r, z, t) = C_{a, 2}(z, t); \quad t \leq t_0$$

$$C_a(z, t) = C_{a, 2}(z, t) - C_{a, 2}(z, t - t_0); \quad t > t_0$$

By use of equations (18) and (11), we obtain the approximate solution for the concentration in the macropore as

$$C_m(z, t) \cong C_0 \exp\left(-\frac{\theta_a D_m z}{r_m^2 \theta_m v_m}\right) \text{erfc}\left[\frac{\theta_a \sqrt{D_a R_a}}{r_m \theta_m v_m \sqrt{t - z R_m / v_m}}\right]; \quad t \leq t_0$$

$$C_m(z, t) \cong C_0 \exp\left(-\frac{\theta_a D_m z}{r_m^2 \theta_m v_m}\right) \begin{cases} \text{erfc}\left[\frac{\theta_a \sqrt{D_a R_a z}}{r_m \theta_m v_m \sqrt{t - z R_m / v_m}}\right], \quad t > t_0 \\
\text{erfc}\left[\frac{\theta_a \sqrt{D_a R_a z}}{r_m \theta_m v_m \sqrt{t - t_0 - z R_m / v_m}}\right] - \text{erfc}\left[\frac{\theta_a \sqrt{D_a R_a z}}{r_m \theta_m v_m \sqrt{t - t_0 - z R_m / v_m}}\right] \end{cases}$$

Equations (34) and (35) are similar to an exact solution developed by Rahman et al. [2004] for analyses of solute transport in a planar macropore surrounded with a matrix.

Similarly, the approximate solution for the matrix is given by
\[ C_a(r, z, t) \cong \frac{C_0}{r} \left( \frac{-\theta_a D_a z}{r_m^2 \theta_m v_m} \right) \text{erfc} \left[ \frac{2 \theta_a \sqrt{D_a R_a} z/(r_m \theta_m v_m) + (r - r_m) \sqrt{R_a/D_a}}{2 \sqrt{t - z R_m/v_m}} \right] ; \ t \leq t_0 \]  

\[ C_a(r, z, t) \cong C_0 \sqrt{\frac{r_m}{r}} \left( \frac{-\theta_a D_a z}{r_m^2 \theta_m v_m} \right) \text{erfc} \left[ \frac{2 \theta_a \sqrt{D_a R_a} z/(r_m \theta_m v_m) + (r - r_m) \sqrt{R_a/D_a}}{2 \sqrt{t - z R_m/v_m}} \right] - \text{erfc} \left[ \frac{2 \theta_a \sqrt{D_a R_a} z/(r_m \theta_m v_m) + (r - r_m) \sqrt{R_a/D_a}}{2 \sqrt{t - t_0 - z R_m/v_m}} \right] ; \ t > t_0 \]  

3. Comparison of Exact and Approximate Solutions

The three cases’ analytical solutions were simulated for different scenarios. We plotted the solutions in dimensionless forms to analyze in a more methodological way. Equations (1) and (2) can be rewritten in terms of dimensionless variables by substituting \( t^* = D_a t / (R_a r_m^2) \), \( r^* = \frac{r}{r_m} \), and \( z^* = D_a z R_m / (r_m^2 R_a v_m) \), which leads to

\[ \frac{\partial C_m}{\partial t^*} = -\frac{\partial C_m}{\partial z^*} + \alpha \frac{\partial C_a}{\partial r^*} \bigg|_{r^* = 1} \]  

\[ \frac{\partial C_a}{\partial t^*} = \frac{1}{r^*} \frac{\partial}{\partial r^*} \left( r^* \frac{\partial C_a}{\partial r^*} \right) \]  

where \( \alpha = 2 \theta_a R_a / (\theta_m R_m) \) and the equations are defined at \( 0 < t^* < \infty, \ 1 < r^* < \infty, \ 0 < z^* < \infty \).

Figure 4.2 shows spatial and temporal variation of concentration for instantaneously released unit solute mass into a macropore (Case 1). The maximum solute concentration in the macropore (\( C_m \)) being large near to the injection point (\( z^* = 0.1 \)) decreases as \( z^* \) increases. As \( t^* (z^*) \) increases, \( C_m \) decreases slowly with a long tail (Figure 4.2a) because of the diffusion occurring between the matrix and macropore. The contaminants in the macropore migrates in radial direction diffusing into the matrix, \( C_a \) concentration.
in the matrix decreases with $r^*$ and $t^*$ (Figure 4.2). Figure 4.2 shows that approximate solutions for case 1 appears to be very accurate for small values of dimensionless time ($t^*$) and distance ($z^*$).

Behaviors of the Case 2 solutions (constant concentration source) are presented in Figure 4.3. Figure 4.3 indicates growing deviations of approximate from exact solutions with increasing $t^*$ and $z^*$. Based on our numerical tests, the Case 2 approximate solutions for both the macropore and the matrix can be used accurately for $t^* \leq 1$ with an error less than 5%.

The results of simulating Case 3 (pulse type) are shown in Figure 4.4. Figure 4.4a shows variation of the normalized solute concentration ($C_m/C_0$) with dimensionless time $t^*$ at specific values of $z^* = 0.1, 0.5$ and $1.0$. $C_m/C_0$ increases sharply until the contaminant front coincides with $z^*$ points of observations. As in Case 1, following the removal of the source from the macropore, solutes initially diffused into the macropore diffused back to the macropore which resulted in a long tailing concentration decrease (Figure 4.4a). Although the Case 3 approximate solutions appear to be in good agreement with the exact solutions for the dimensionless pulse time chosen as $t_0^* = 0.5$ (Figures 4.4a-b), the error grows with increasing $t_0^*$ as can be seen from Figure 4.5.

In Figure 4.2-4.5, the concentrations are plotted for different values of $t^*$ and $z^*$ keeping $\alpha$ (=1.4) at a constant value. Effect of $\alpha$ on the concentration at the macropore wall ($r=r_m$) is demonstrated for cases 2 and 3 in Figure 4.6. Figure 4.6a shows that the concentration at the pore wall decreases with increasing $\alpha$ when a fixed type concentration boundary condition is applied at top of the macropore (case 2). For case 3
representing the pulse-type boundary condition, a plot of the concentration versus \( \alpha \) shows a bell-shaped curve skewed to the right (Figure 4.6b).

4. Conclusion

Analytical solutions were presented for advective solute transport in a macropore with diffusion into an unbounded soil matrix. The analytical solutions were obtained in integral forms for an instantaneous, fixed and pulse type boundary conditions. We also presented approximate solutions for the all three cases. One can test whether to use approximate or exact solutions if \( a \ priori \) estimates of the parameters are available. The numerical experimentation by varying parameters for a wide range of all parameter values showed that generally, the approximate solution is sufficient for relatively short solute transport times.
LIST OF REFERENCES
References


APPENDIX
Figure 4.1. Schematic demonstration of the geometry of the macropore-matrix system
Figure 4.2. Comparison of the exact and approximate solutions for spatial and temporal variation of the solute concentration in a) macropore and b) matrix at $z^*=0.5$ for Case 1 ($\alpha=1.4$).
Figure 4.3. Comparison of the exact and approximate solutions for spatial and temporal variation of the solute concentration in a) macropore and b) matrix at $z^*=0.5$ for Case 2 ($\alpha=1.4$).
Figure 4.4. Comparison of the exact and approximate solutions for spatial and temporal variation of the solute concentration a) in macropore, and b) in matrix at $z^*=0.5$ for Case 3 ($\alpha=1.4$ and $t_0^* = D_u t_0/ (R_o r_m^2) = 0.5$).
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PART V
DEVELOPMENT OF A MOISTURE MOMENT METHOD TO MEASURE UNSATURATED SOIL PROPERTIES
Abstract

A moisture moment method is presented to collect and analyze data for estimating a soil’s water retention and unsaturated hydraulic conductivity functions. An initially dry soil column is suspended horizontally at each end by a load cell. Water is slowly imbibed at one end of the soil column. The water pressure at the inlet and the change in load measured by each load cell are measured throughout the test, which is sufficient to estimate the soil’s unsaturated soil hydraulic properties. We applied the method to a 14.5-cm long by 3.65-cm diameter sandy silt loam soil. The test was completed within a period of 2 hours. The estimated water retention curve was compared to that measured using a Gamma Ray attenuation system that was run concurrently during the moment testing protocol. Results from the preliminary testing of the method are promising.

1. Introduction

Determination of soil hydraulic properties (i.e., the functional relationship among water content-pressure head-hydraulic conductivity or hydraulic diffusivity) is required, along with initial and boundary conditions, to track fluid and solute retention and movement in unsaturated porous media. Traditional methods to measure basic soil hydraulic functions are time consuming and expensive. Most steady-state based methods require weeks to months to complete. The dynamic methods typically solve for the functions inversely and require a relationship between the water retention and hydraulic conductivity functions, such as the van Genuchten-Mualem relationship (van Genuchten, 1980). Often, difficulties with solution uniqueness arise (Vachaud et al., 1972; Toorman et al., 1992). More recently, geocentrifuges have been used to measure the hydraulic
functions quickly by imposing extreme pressure gradients within small soil samples (Simunek and Nimmo, 2005), but the analysis remains quite expensive.

Measurement of the unsaturated hydraulic conductivity by incorporating a moment measurement was first proposed by Zaslavsky and Ravina (1965) and named as the moisture moment method. By use of Darcy’s law and the continuity equation, Zaslavsky and Ravina (1965) derived a general equation describing the change in moment for 1-D horizontal imbibition. Youngs (1968) also used this method to estimate sorptivity of soils. Since 1968, to our knowledge the method has not been used or improved until Tyner et al. (2006) recently applied it to the hot air method used to measure soil hydraulic diffusivity described by Arya (1975). These previous methods did not attempt to measure soil tension and construct the water retention curve. Measurements of soil suction using porous sensors generally suffer from long equalization times and are confined to less than 100 kPa because of cavitations problem occurring in measuring systems (Gee et al., 2002; Agus and Schanz, 2005).

We present an improved moisture-moment method to collect and analyze raw data in an inexpensive, rapid and accurate manner that also yields the water retention curve.

2. Background Theory

Conservation of mass for water content in a horizontal one-dimensional porous medium is expressed by

\[ \frac{dq}{dx} = -\frac{\partial \theta}{\partial t} \]  \hspace{1cm} (1)
where \( q \) is the water flux (cm/s), \( \theta \) is the water content (cm\(^3\)/cm\(^3\)), \( x \) is the distance from the inlet boundary (cm), and \( t \) is time (s). Multiplying both sides of Eq. (1) by \( x \) and integrating from \( x=0 \) to the end of the column position, \( x=L \), we obtain,

\[
- \int_0^L q \, dx = - \int_0^L x \frac{\partial \theta}{\partial t} \, dx \tag{2}
\]

Using Darcy’s law, \( q \) can be expressed as

\[
q = -K(h) \frac{\partial h}{\partial x} = -D(\theta) \frac{\partial \theta}{\partial x} \tag{3}
\]

where \( h \) is the matric potential (cm), \( K \) is the hydraulic conductivity (cm/s) as function of \( h \), and \( D \) is the hydraulic diffusivity (cm\(^2\)/s) defined as \( D(\theta) = K(h) d\theta/dh \). \( \theta \) is a function of \( h \), and this functional relationship is used to construct the water retention curve. By substituting the \( K(h) \) version of Eq. (3), Eq. (2) becomes

\[
\int_{h_0}^{h_i} K(h) \, dh = - \int_0^L x \frac{\partial \theta}{\partial t} \, dx \tag{4}
\]

where \( h_i \) is the matric potential at the inlet boundary, and \( h_0 \) is the initial matric potential. \( K \) can be represented as a power series:

\[
K(h) = \sum_{i=0}^{\infty} c_i/h^i \tag{5}
\]

where \( c_i \) is defined by \( c_i = 1/i! (\partial^K K/\partial h^K)_{h=0} \). Substituting Eq.’s (5) into Eq. (4), followed with term by term integrations leads to:

\[
c_0' + c_0 h_i + c_1 \ln h_i - 2 c_2 \frac{1}{h_i} - 3 c_3 \frac{1}{h_i^2} + ... = \int_0^L x \frac{\partial \theta}{\partial t} \, dx \tag{6}
\]

where \( c_0' \) is a function of initial matric potential.
In the following sections, we will describe an experimental technique to make use of Eq. (6), which gives the relationship for the time rate of change of moment, and the initial and inlet pressure so that unsaturated hydraulic conductivity can be calculated as function of tension.

3. The Measurement of Soil Hydraulic Properties by the Moisture Moment Method for the Horizontal Infiltration Tests

A homogenous column/core approximately 14.5 cm long with a soil at an initially low water content, \( \theta_0 \), is hung from two load cells as shown in Figure 5.1. A water pressure sensor is attached to the inlet to measure \( h_i \). On the contrary to the hot-air method and Bruce-Klute test, the boundary condition for water content inlet need not be constant. The test begins with a large tension imposed on the inlet, and the tension is decreased gradually during the testing period. A data logger records the cumulative change of force acting on each load cell during the wetting period, \( \Delta F_1(t) \) and \( \Delta F_2(t) \), and \( h_i(t) \). The cumulative volume of water added, \( V_w(t) \), is given by

\[
V_w(t) = \frac{\Delta F_1(t) + \Delta F_2(t)}{\rho_w g} = \int_0^L \int_0^R \Delta \theta(x,t) r dr d\phi dx \tag{7}
\]

where \( \theta(x,t) = \theta(x,t) - \theta_0 \). Moment of the cumulative change of forces, \( \Delta M \), around the inlet, \( x=0 \) renders

\[
\Delta M = \rho_w g \pi R^2 \int_0^L x \Delta \theta(x,t) dx \tag{8}
\]

where \( L \) is the distance to the load cell # 2 (see Figure 5.1). The derivative of Eq. (8) with respect to time gives
\[
\frac{1}{\rho_w g \pi R^2} \frac{dM}{dt} = \int_0^l x \frac{\partial \theta}{\partial t} dx
\]

(9)

where \( \theta(x,t) \) is equal to zero for \( x \geq x_{wf} \) (wetting front position). Eq. (9) was first proposed by Zaslavsky and Ravina (1965). Substituting Eq. (9) into Eq (6), we obtain the required relationship between the change in moment measured versus the initial and inlet tension as function of time:

\[
c_0 \ ln h_i + c_1 \ln h_i - 2c_2 \frac{1}{h_i^2} - 3c_3 \frac{1}{h_i^2} + ... = \frac{1}{\rho_w g \pi R^2} \frac{dM}{dt}
\]

(10)

Eq. (10) becomes invalid if water exits the column. The derivations listed from Eq. (4) to Eq. (9) can also be expressed in terms of \( D \) and \( \theta \). Using multiple measurements of \( dM/dt \) versus \( h_i \) or \( \theta_i \) through time, and by solving via nonlinear regression or a standard least-square procedure after linearization, we obtain the coefficients \( c_0, c_1, c_2, ... \). Then, using the power series representation, \( K(h) \) can be calculated.

3.1. Construction of the Water Retention Curve Function

One can estimate unsaturated hydraulic conductivity \( K \) from Eq. (5) with the help of Eq. (10) from measurements of \( dM/dt \) and matric potential, \( h_i \), at different times. Estimation of \( \theta_i \) versus measurement of \( h_i \) provides the water retention curve function. One way to achieve this is to propose an empirical type equation for water content distribution and substitute it into both Eq. (7) and Eq (8), and the resulting equations can be used simultaneously to estimate the unknown parameters of the empirical equation from the measured load cells data (Tyner et al., 2006). Then, by this approach \( \theta_i \) at any time can be computed. In this section, we propose a simple algorithm to estimate \( \theta_i \) as function of time.
The water content distribution through the column at any time can be defined by using a test function which satisfies the following boundary conditions

\[ \theta(0,t) = \theta_i(t), \quad \theta(\text{w}_{\text{f}},t) = \theta_0 \]  

(11)

As an example, the following function satisfies Eq. (11) and has one unknown parameter, \( a \):

\[ \theta(x,t) = \theta_i(t) - \left[ \theta_i(t) - \theta_0 \right] \exp \left[ \frac{x - \text{w}_{\text{f}}}{a} \right]; \quad a \geq 0, 0 \leq x \leq L \]  

(12)

After substituting Eq. (12) into Eq.’s (7) and (8) and rearranging, we obtain:

\[ \frac{\Delta M(t)}{\Delta F_1(t) + \Delta F_2(t)} = \frac{\int_0^{\text{w}_{\text{f}}} x \{1 - \exp \left[ a \left( x - \text{w}_{\text{f}} \right) / x \right]\} \, dx}{\int_0^{\text{w}_{\text{f}}} \{1 - \exp \left[ a \left( x - \text{w}_{\text{f}} \right) / x \right]\} \, dx} \]  

(13)

Then, evaluation of the integrals above leads to

\[ \frac{\Delta M(t)}{\Delta F_1(t) + \Delta F_2(t)} = \frac{\text{w}_{\text{f}}}{2} \left[ -a + \frac{\exp (-a)}{\Gamma(0,a)} \right] \]  

(14)

where \( \Gamma(0,a) \) is the incomplete gamma function. By using the data obtained from the load cells at specific times, \( a \) can be calculated inversely from Eq. (14) for each specific time. This can be achieved easily by using commercial math softwares such as Mathematica, Matlab, etc. Once values of \( a \) have been calculated, \( \theta_i \) can be found from

\[ \theta_i(t) = \theta_0 + \frac{1}{\rho g \pi R^2} \frac{\Delta F_1(t) + \Delta F_2(t)}{a \exp (a) \text{w}_{\text{f}} \Gamma(0,a)} \]  

(15)

where \( \theta_0 \) must be measured before the beginning of the test. By combining suction measurements recorded at the same periods with the water content estimations, water retention curve can be constructed. As a verification of this approach, water content
measurements recorded from a gamma ray attenuation system will be compared with the estimated water content values by Eq. (15). It should be noted that the function, Eq. (12), with one parameter, \( a \), is only one of the suitable functions which satisfy the boundary conditions.

4. Experimental Setup

In this section, we describe an experimental setup that is designed to measure unsaturated hydraulic properties. We hang the soil column horizontally from two load cells, which are connected to a data logger (Figures 5.2). One end of the soil column is attached to a porous ceramic plate. The ceramic plate is connected to a water reservoir system that provides water to the soil inlet at a desired tension. A pressure transducer connected to the water reservoir records tension at the inlet (Figure 5.2). By use of a Gamma Ray attenuation system described in Tyner et al. (2005), the change in water content has been measured, which are used to validate our new testing method. We applied the method described in Section 4 to a 14.5-cm long by 3.65-cm diameter sandy silt loam soil column. The soil was hand packed into a transparent column. Water was allowed to enter to the soil column by decreasing the inlet tension from nearly 0.5 bar to 0.09 bar tension over a period of 2 hours.

5. Results

The rate of change in moment is shown in Figure 5.4a. A nonlinear regression was applied to the curve to obtain the coefficients \( c_i \) of Eq. (10). As the degree of the polynomial type equation, Eq. (5), increases, precision for estimation of \( K \) increases. Based on our experiences with testing the approach, a third or fourth order approximation
is typically sufficient to accurately estimate $K$. The resulting unsaturated hydraulic conductivity given by Eq. (5) is plotted for the suction interval measured during the testing (Figure 5.4b).

The individual values of $a(t)$ were calculated inversely from Eq. (14) (see Table 5.1). Then, Eq. (15) was applied to calculate the water content at the inlet. With the known values of $a$ and $\theta_i$, the water content profile was plotted as function distance from the inlet (Figure 5.5).

As a validation of the approach described above for constructing water retention curve function, water content measurements were recorded simultaneously using a custom gamma-ray attenuation system described in Tyner et al. (2005). A gamma-ray system is not required to conduct our proposed method and was only used for validation. Figure 5.6 presents a comparison of measured water contents by the gamma-ray system and the calculated water content values from Eq. (16).

6. Conclusions

We presented an moisture moment method that allows estimation of soil hydraulic functions by analyzing the moment created by 1-D imbibition along within inlet water tension, both as a function of time. The method was tested on a sandy silt loam during a 2 hour test. Unsaturated hydraulic conductivity was computed from dry conditions (~400 cm suction) up to near saturation (~90 cm suction). The water retention function was also obtained. A Gamma Ray attenuation system was used to validate the water retention function predictions and showed very favorably comparison.
References


APPENDIX
Table 5.1. Calculation of parameter a and water content at the inlet.

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<th>( t ) (min)</th>
<th>( x_{nf} ) (cm)</th>
<th>( \frac{\Delta M}{\Delta F_1 + \Delta F_2} ) (cm)</th>
<th>( a ) by Eq.(15)</th>
<th>( \theta_i ) (cm(^3)/cm(^3))</th>
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</tbody>
</table>
Figure 5.1. A load cell suspends each end of a soil column. Imposed on the soil column is a graph of moisture content versus distance from the wetting face, $\theta(x, t)$. The gray area above represents the change in moisture content since wetting began and it is proportional to cumulative volume of water added.
Figure 5.2. Simplified schematic of the experimental setup
Figure 5.3. Gravimetric changes in load cells versus time
Figure 5.4. Demonstration of time rate of change in moment and estimation of $K(h)$ curve.
Figure 5.5. Estimated water content profiles computed at different times.
Figure 5.6. Water content measurements with Gamma Ray and comparison with estimated water retention.
VITA

Abdullah Cihan was born in Ankara, Turkey, 1980. He graduated from High School, Ankara Gazi Ciftligi Lisesi, in 1996. He received his bachelor degree from Department of Geological (Hydrogeology) Engineering at Hacettepe University, Ankara, in 2002. He received a master degree from Department of Geological Engineering at Middle East Technical University, Ankara, in 2004. He is currently pursuing his doctorate program in Biosystems Engineering and Soil Science at University of Tennessee.