Determination of Soil-Water Characteristic Curve Using Percolation in Multifractal Media

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Abstract
The relation between volumetric water content and water potential for a soil is termed its Soil-Water Characteristics Curve (SWCC). This basic hydraulic property is closely related to the soil pore size distribution. In this study, basic soil parameters are used to develop a multifractal model of soil structure. After arriving at the most suitable fractal medium which is a multifractal one, the corresponding pore characteristics are implemented in a percolation network to calculate SWCC. Finally, a comparison is made between results obtained from the proposed model and the real soil behavior.
Keywords: Fractal, Percolation, Soil -Water Characteristic Curve, SWCC

Introduction

Unsaturated soil mechanics has gained wide applications in geotechnical engineering practice. Soil behavior in its saturated state is far from its unsaturated condition. However, the implementation of unsaturated soil mechanics into engineering practice depends to a large extent upon the ability to estimate unsaturated soil properties. The soil-water characteristic curve has proven to provide a satisfactory tool to estimate basic mechanical properties of unsaturated soils. Soil-Water Characteristic Curve (SWCC) displays the relation between volumetric water content and water potential for a soil.

It has long been recognized that the behavior of water in soils depends on pore space geometry. Quantification of this geometry by means of fractal concepts offers an opportunity to relate soil water properties to the soil basic structural properties. Fractal objects exhibit three defining attributes: similar structure over a range of scales, intricate structure that is scale independent, and irregular structure that can not be captured entirely by classical (i.e., Euclidian) geometrical concepts, necessitating, for example, the use of a spatial dimension that is not an integer, [1]. Like the mathematical objects in Euclidian geometry, circles, spheres, cones, or cubes, the objects in fractal geometry are idealizations that can only approximate the pore scale structures encountered in natural soils, but nonetheless they are useful to represent some of the inherent complexity in these porous media. Fractals are divided into two specific categories based on their complexity of the structure and similarity of the repeated pattern inside them. These two categories are mono-fractals and multifractals. Mono-fractals can be readily defined by one parameter which is their fractal dimension whereas multifractals are more complicated and usually defined by a spectrum instead of only one dimension. Multifractal are more natural and utilizing them in modeling involves less simplification and more accuracy. So far, most researchers have preferred to model soil as a mono-fractal and measuring fractal dimension of grain size distribution for estimating required parameters in empirical equations of SWCC. Casting a glance on all models which have been presented to date, the question arises whether these models are precise enough to determine the SWCC or there is still a need to improve these models. This task can be achieved through consideration of multifractals instead of mono-fractals and by changing the current approach from direct usage of the fractal dimension to the application of pore characteristics obtained from multifractal simulation of soil. To relate mathematically the soil-water properties to pore arrangement within the soil and its pore size distribution percolation theory should be employed. Though percolation theory has played a great role in recent researches in ground water hydrology, hydrogeology, and soil mechanics, few researchers have employed it in conjunction with a multifractal soil model. Percolation theory can be considered as a complementary method to take the most advantage of multifractal modeling. Application of a percolation approach can provide us with a

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suitable tool in taking soil pores into account and multifractal models can serve as a bridge between soil parameters and its structure; they can provide better understanding of the soil heterogeneity and yield the pore size distribution required for implementation in the percolation approach. Hence, a joint approach of multifractal modeling and percolation theory can cover all aspects of such modeling.

Considering all aforementioned statements about SWCC modeling, present study was conducted in three phases. First, after investigation of current fractals the most suitable fractal media was generated such that it had the same porosity and particle size distribution as the real soil and it was used to compute the soil pore size distribution. Next, a percolation network was constructed. This was achieved by randomly placing pores with different sizes on the nodes of a network and after that, percolation theory was applied to control the drainage of the network at successive suctions. These stages are described in more details in the subsequent sections of this paper and the results of the proposed approach are compared with those of real soil behavior.

From early empirical models to the multifractal approach

Several empirical models have been proposed in the literature which link, by means of multiple regression technique, water content, for an assigned water potential value to different soil parameters: texture, organic matter, bulk density, etc. [2]. Various authors (Arya and Paris, 1981; Haverkamp and Parlange, 1986; and Mishra et al., 1990) have proposed physically based models that use the well-known relations between pore diameter and water potential and deduce pore distribution from the distribution of the particle diameter, [3,4,5]. In particular, Arya and Paris's model considers soil as a medium consisting of a set of spherical particles and cylindrical capillaries, each characterized by a volume that is dependant on particle diameter, the gravimetric fraction of particles belonging to a given class of diameters, and an empirical coefficient α obtained through a nonlinear regression method between the measured and calculated values.

Given the complexity and irregularity of the porous system, in the past few years, the fractal approach introduced by Mandelbrot, has been employed to characterize the irregular and complex geometry of the soils. Studies are now available, showing that classical data on soil structure can be interpreted in terms of fractal geometry. For example, either particle-size distribution [6] or pore number-size distribution of soils [7], as well as mass-size distributions measured in aggregated soils, [8], often fit power laws whose exponent may be interpreted in terms of a fractal dimension that can be related to main soil characteristics. Pertinent to the above approaches are also several studies that indicate additional promise in relating the cumulative size distribution to the SWCC. In one case, fractal theory and scale invariance properties are used to show that the empirical coefficient α, in the Arya and Paris model, is equivalent to the fractal dimension of a tortuous fractal path of pores,[9,10].

It was not common to consider multifractal models for soil structure until recently, when Perfect et al., 2006, used a simple multifractal model to investigate soil saturated hydraulic conductivity. Though, multifractals can include details of soil particle-size distribution. They did not adjust their model parameters with basic soil parameters like particle-size distribution and soil porosity. Their only emphasis was on its flexible use and their objective was to determine saturated hydraulic conductivity by means of a multifractal spectrum which is a spectrum of singularities characterizing all the information hidden inside a multifractal at different scales, [11]. In the present study in order to make more flexibility in the model of Perfect et al., which was a deterministic multifractal; the model is changed to a random one. It is of crucial importance to use each fractal model in its right place. Whereas deterministic fractals can be found in some natural objects, it seems better to consider soil medium as a random multifractal medium since each pore or particle can be found everywhere in the medium and the connection and position of soil pores may not follow a simple mathematical rule, necessarily. There are enough degrees of freedom in placing pores within a random multifractal and producing particles of different sizes as required to facilitate model adjustment to the basic soil parameters. Moreover, since the results from 2-dimensional modeling were not satisfactory, a 3-D random multifractal model was created and used.

Gouyet Random Multifractal Model

The random multifractal used in the present study was obtained by considering the necessary modifications in the famous Gouyet random multifractal model, [12]. Gouyet random multifractal model is generated by the following algorithm:

- Divide the initiator into b^2 parts.
- Choose probability p (=1-n/ b^2) that b^2-n parts remain
- Generate random numbers in [0 1] interval and assign them to each part.
- If the generated number is greater than zero it will be deleted in the next iteration (assign zero to that cell)
- Else assign one

Let us study the behavior of this algorithm. Assume that we wish to generate a random multifractal following the Gouyet algorithm. Assuming b=3 and p=0.5, the generated multifractal after the first iteration will be as illustrated in Figure 1, and after the second iteration as shown in Figure 2.

0.9501	0.4860	0.4565
0.2311	0.8913	0.0185
0.6068	0.7621	0.8214

(a)

0	1	1
1	0	1
0	0	0

(b)

Figure 1- Random multifractal after first iteration (a) the primary assigned random numbers, (b) generated multifractal

0	0	0	0.4447	0.9218	0.4057	0.4103	0.3529	0.1389
0	0	0	0.6154	0.7382	0.9355	0.8936	0.8132	0.2028
0	0	0	0.7919	0.1763	0.9169	0.0579	0.0099	0.1987
0.8462	0.6721	0.6813	0	0	0	0.6038	0.0153	0.9318
0.5252	0.8381	0.3795	0	0	0	0.2722	0.7468	0.4660
0.2026	0.0196	0.8318	0	0	0	0.1988	0.4451	0.4186
0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0

Figure 2- Random multifractal after second iteration

Ones are considered as pores and zeros as particles of the soil medium. It is worth noting that this matrix can be regarded as a black and white image of a section of soil. In a programming language like MATLAB, ones become white pixels and zeros form the black pixels depicting particles body and boundary.

Proposed Random Multifractal Model

To create a more realistic model of soil, this simple algorithm should be modified to tune with real soil conditions. Thus, p should be reasonably selected such that the particle size distribution is satisfied. The final algorithm has the following steps:

- Consider a set D of the soil grain sizes ,such that:

$$D = \{d_i \mid d_i \in Soil\ Grading\ \&\ d_i / d_{i-1} = k\} \qquad (1)$$

where k is a constant integer number.

- Make the initiator to satisfy the void ratio criteria. In this step void ratio of the soil is implicitly used to make the representative soil volume (total area of the fractal model if the model is 2-dimensional or its total volume if the model is 3-dimensional). When the particle size distribution of the model converges to the required values and with the void ratio implicitly considered in the construction of model, the model will be tuned with the basic soil characteristics. The total area (in the case of 2-D fractals) or total volume (in the case of 3D fractals) which is denoted by V_I , will be calculated from Equation 2.

$$V_I = (\sum_{i=1}^{n} v_i)(1+e) \qquad (2)$$

where e is the soil void ratio and n specifies the number of grain size classes present in the set D.

- In the first iteration: Produce the random numbers and check them with the threshold value p_1 where p_1 is defined by :

$$p_1 = 1 - \frac{1}{1+e} = m \tag{3}$$

where m is the soil porosity.

- Note that in the first iteration the number of the segments is selected such that the unit cell size of the fractal matches the maximum grain size included in the set D.
- As long as particle size distribution is not satisfied, the threshold probability value is modified according to Equations 4 and 5.

$$p_{new} = p_{old} + \Delta p \tag{4}$$

$$\Delta p = (n_i - ng_i) / n_T \tag{5}$$

where, i is the iteration stage number and n_g is the total number of grains having the current cell size of the fractal medium derived from the soil particle size distribution curve.

Remark: Note that the CDF (Cumulative density function) behind random generators in not decreasing, therefore, it is evident that G(x) = (1-CDF(x)) is decreasing. With a drop in p (threshold value), the probability in which one may face random numbers greater than p will increase. If $n_i > ng_i$ then Δp will be negative and hence, the number of the cells containing random numbers greater than p will increase so that there will be greater number of pores and thus number of particles will decrease to reach the value obtained from particle size distribution curve (PSD) of the soil. It means that each stage of this algorithm has a kind of iterative structure to satisfy PSD of the soil.

- Repeat the algorithm for the subsequent stages, divide cells containing zeros into k subcells, fill them with random generated numbers and find the best matching threshold probability value.

It is important to enhance the speed of convergence by selecting appropriate probability values for the initial threshold values; in this regard the first threshold value in each stage is the last one of the previous stage. As it was stated previously, in the present study after investigating capabilities of 2-D random multifractals and arriving at their deficiencies to model the soil structure satisfactorily, 3-D random multifractals were generated and used. There is no big difference between the algorithms of creating 2-D and 3-D multifractals; the only difference is the medium dimension and notations used to define the procedure. As mentioned before, in the case of 3-D modeling the total volume of the model is computed by summing the corresponding volumes of particles in set D using Equation 2.

Extraction of the soil pore size distribution

There are several 3D morphological image processing techniques which most of them are developed and improved by Lindquist and his colleagues at State University of New York (SUNY) for pore network reconstruction purposes. Such algorithms assign numbers to the cells of the pore regions so that they can find pore centers by searching local maxima among assigned numbers [13]. In the present study *bwlabeln* function of the image processing toolbox in MATLAB version 7.0.0.19920, (R14), was modified and used for this objective. This function can label connected components in N-D binary image. The main point in its use was to define suitable connectivity matrix. Here, different groups of the 3-D pixels with the same value – e.g., 1: representing pixels of a pore region - will be considered connected if they have common faces. Actually, this procedure is based on searching for minimum connections among the groups of pixels to separate them into individual pores and particles.

Percolation theory

Pores extracted from the previous stage were implemented in a 3-D network and percolation theory was employed to obtain the SWCC. In this section a straightforward introduction to the basic concepts of percolation theory is presented.

The mathematical percolation theory can be employed to investigate the transition of two different phases, i.e., wetting and non-wetting phases, through a soil porous medium. This theory was developed in statistical physics, [14]. Lowry and Miller (1995) developed an approach, which provided a 3-D network with random connectivity, [15]. With the pore size distribution obtained from multifractal model, the SWCC can be determined using relationship between soil suction and radii of pores. In such models, investigation of the correlation between the neighboring pores and throats is necessary to find a continuous path of dewatering, for a certain level of suction. At the beginning, the constructed pore network is full of water, as it is in the saturated condition of real soil. Then by applying successive suctions, pores become dewatered and water content of the network at each level of suction can be computed. Here, pore bodies are assumed to be spherical to simplify the model. In the percolation networks, a throat is usually considered with a certain diameter between the two neighboring pores. The relationship between size of end pores and throats has been studied by Mohanty and Salter (1982) and Li et al., (1986), [16,17]. Percolation theory can be considered as a suitable tool in computation of unsaturated soil characteristics, for example, some researchers employed percolation theory for determination of effective stress parameter in unsaturated soils, [18].

Proposed Percolation Model

To generate the conceptual percolation model the following procedure was perused:

1. Pores obtained from 3-D image processing of the random multifractal model were distributed randomly on the nodes of a 3-D network.
2. A throat was considered, between each pair of adjacent nodes. As revealed by other researchers, an appropriate relation between diameter of the end pores and that of throat can be expressed in the form of Equation 6.

$$d_{th} = f(d_{p1}, d_{p2}) = C.d_{\min} \quad (6)$$

Since in real soils throats of different sizes are distributed randomly, it is not reasonable considering only one coefficient to produce all throats. In the present study, based on random generated numbers which can belong to different probability intervals, a sequence of coefficients were produced and used to generate the throats.

3. For different levels of suction, the network becomes dewatered and the drainage curve can be estimated. In each level of suction the minimum throat diameter which controls dewatering of its adjacent pores can be calculated from Kelvin's capillary model for surface tension as follows:

$$r_i = \frac{2T_s \cos\alpha}{\psi_i} \quad (7)$$

where, T_s is water surface tension, ψ_i stands for the applied suction level, α specifies the contact angle and r_i denotes the corresponding minimum throat radius. Now, a search is performed and wherever throat diameter is greater or equal to this value, end pores and throat become dewatered. An exception is made to provide a continuous path of drainage, i.e., in the interior layers of the network it is considered necessary to have one end node dewatered in addition to the aforementioned criteria to dewater the throat and the other end pore. This additional statement provides continuous paths of drainage throughout the network. Schematic illustration of the percolation network is depicted in Figure 3.

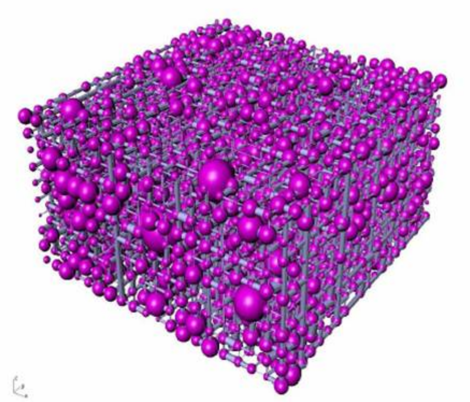


Figure 3– A schematic illustration of the percolation network

Implementation Remarks

The above-mentioned stages were coded in the MATLB environment. All pores which drain at indifferent suctions can be placed in a single network, provided that enough RAM memory is available for computation. Since MATLAB makes arrays in a manner that they occupy much more memory than it is usually needed in other environments. The percolation network was divided into sub-networks which, in some cases, led to anomalies in the results. Improvement and enhancement of the results may be fulfilled by defining a specific way of memory allocation in MATLAB, utilizing dynamic programming or other sophisticated methods.

Results and Discussion

Experimental results reported by various researchers and compiled by Soil Vision Database have been used to investigate the suitability of the proposed approach and its scope of application. Figures 4 and 5 show typical 2-D and 3-D multifractals that can be generated using the proposed approach.

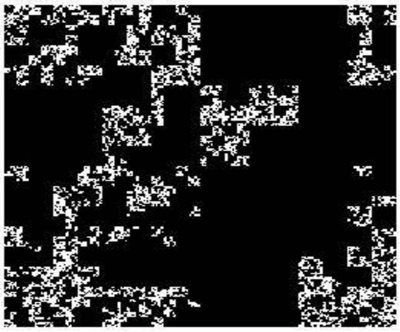


Figure 4– Typical 2-D random multifractal model for soil generated by proposed approach

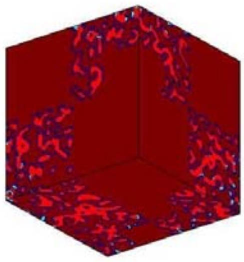
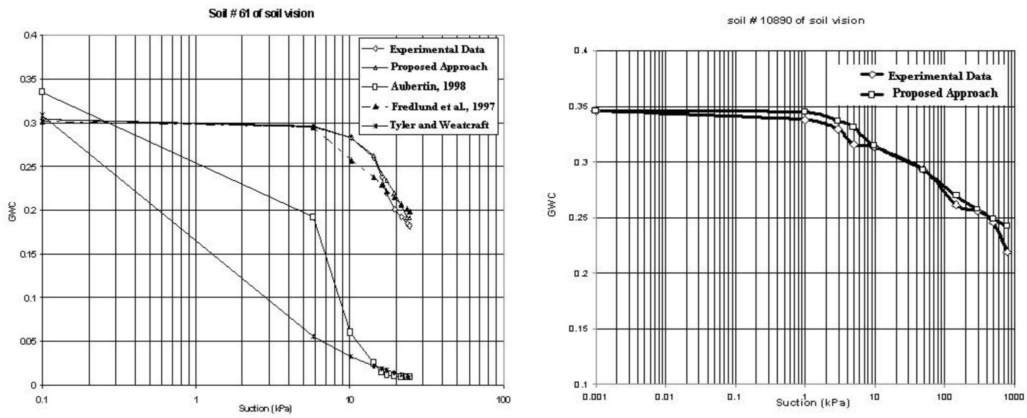


Figure 5– Typical 3-D random multifractal model for soil generated by proposed approach

Figures 6 through 8 indicate three categories of SWCCs simulated using the proposed approach and compared with the experimental results. To investigate suitability of this approach a comparison is also made with predictions of other researchers (see Figures 6 (a), 7 and 8).



(a) **(b)**

Figure 6– Simulated and experimental SWCC curve for (a) soil # 61 and (b) soil #10890 of Soil vision

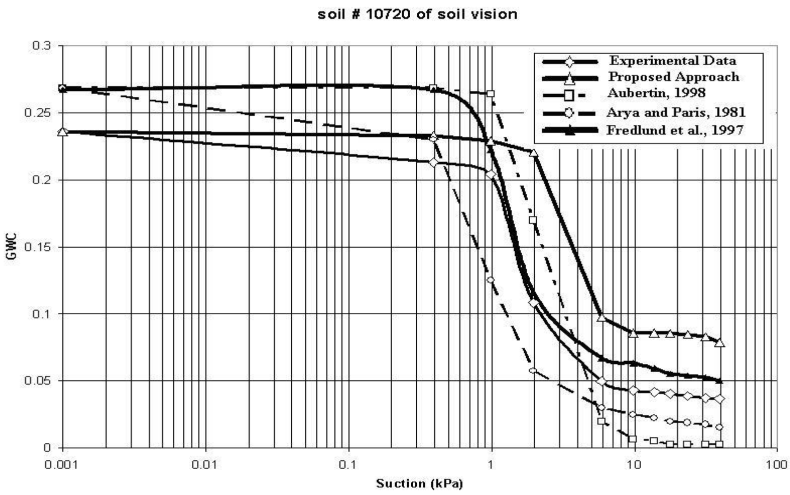


Figure 7– Simulated and experimental SWCC curve for soil # 10720 of Soil vision

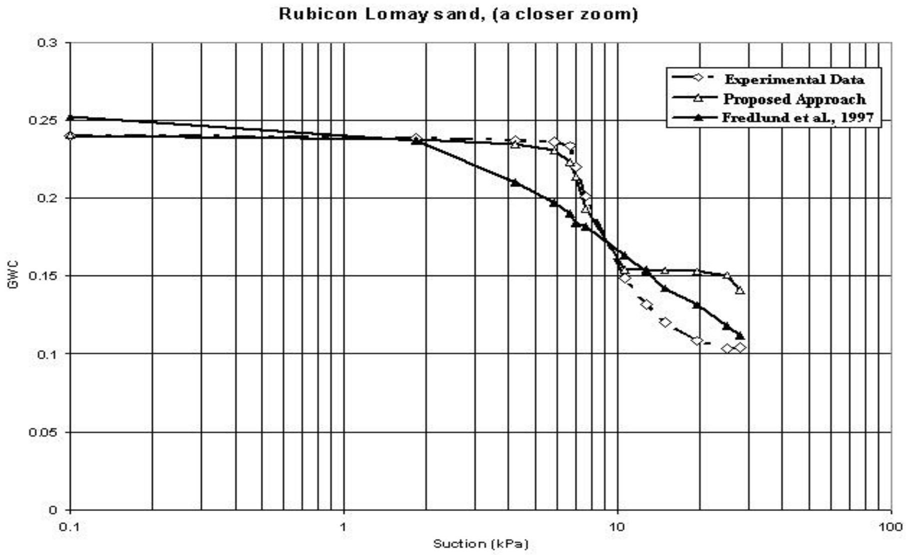


Figure 8– Simulated and experimental SWCC curve for Rubicon loamy sand (soil #63 of soil Vision)

In the first category, the model has simulated SWCC with a reasonable accuracy up to high levels of suction (1000 kPa or so). Soils classified as silts and sandy silts (having a uniform variation in grading) commonly belong to this category of results. In the second category, the predicted SWCCs are overestimated as compared with the real soil behavior. As shown in Figure 7, coarse to medium grained sands usually belong to this group of results. Finally, in the third category of results some anomalies were observed because of placing pores in more than one percolation network. This was required, since the program was run on a personal computer, and the MATLAB environment imposed specific restrictions on the dimension of the network. Hence, a set of connected networks were used each containing a portion of the soil pores. Figure 8 demonstrates a typical anomaly in simulated SWCC. It is noteworthy that enhancing capabilities of the program and solving memory allocation deficiencies may remove such anomalies.

Concluding Remarks

In this paper, multifractal modeling in conjunction with percolation theory was employed to predict SWCC. The results show that the proposed approach can be used to predict SWCC of different soil types though its accuracy is highly dependent on the soil type and its particle size distribution. However, further work is required to enhance accuracy of the results in all suction intervals and for all types of soils. Moreover, the shape of particles generated in the multifractal modeling of the soil can have a remarkable influence on the resulting SWCC especially in the case of very fine grained soils such clays. Last but not the least, the effect of surface charges of soil minerals on the drainage mechanism of water films and pendulars must be included in a more detailed simulation.

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