# Pore-Scale Analysis Using Mathematical Morphology to Obtain Soil Hydraulics Properties

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ABSTRACT: Evaluation of the hysteretic drainage and wetting phenomena exhibited by porous media is relevant to many branches of science and engineering. In subsurface hydrology, these processes play a particularly important role in the vadose zone where the soil is partially saturated with water. In this paper, we focus on the determination of the water retention curve for a porous medium through a novel pore-scale simulation technique that is based on mathematical morphology. Advances in tools for analyzing 2- and 3-D images have made this technique very attractive for elucidating macroscopic relationship from pore-scale analysis. We present an algorithm that allows for the representation of three-dimensional randomly packed porous media of any geometry (i.e. not restricted to idealized geometries such as spherical or ellipsoidal particles/pore space) so that the connectivity-, tortuosity-, and hysteresis-causing mechanisms are represented properly, and their role in determining macroscopic fluid behavior is made explicit. Using this method, we present simulation results that include both drainage and wetting processes, in order to demonstrate hysteretic effects. Entrapment of wetting and non-wetting phases during both drainage and wetting are also represented explicitly. This technique is used to model hysteresis behavior and the relationships between water pressure, saturation and interfacial area. Strengths and limitations of this method are described.

#### INTRODUCTION

The drainage and wetting of porous media are two important phenomena pertinent to many branches of science and engineering, as nearly all materials, whether man-made or naturally occurring, are porous in nature to a certain degree. In subsurface hydrology, these processes play a particularly important role in the vadose zone where the soil is partially saturated with water. When additional immiscible fluids are present, then these principles have to be extended to multiphase flows. Two macroscopic constitutive relationships quantify the processes of drainage and wetting in soils: Water Retention Curve (WRC) that describes the capillary pressure-water saturation relationship, and the relative hydraulic conductivity function that relates the hydraulic conductivity to water saturation. These relationships are significant not only because they provide mathematical descriptions of the processes, but also because they are necessary components in the governing equations that model water flow and contaminant movement in the vadose zone under unsaturated conditions or in multiphase systems.

In this paper, we limit our attention to the determination of the WRC from a porous medium through a novel pore-scale simulation technique that is based on mathematical morphology. Mathematical morphology deals with applications in processing of discrete quantized (pixelized) images in order to extract useful properties of the medium. This branch of mathematics traces its roots to the early works of Serra and Matheron on ore reserve estimation (Serra, 1967) and on permeability of porous media in relation to their geometry (Matheron, 1967). Since Serra (1982) popularized this method, mathematical morphology has been applied primarily to the field of image and video processing despite its early ties to geotechnical and hydrologic engineering. More recently, many new algorithms

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have been developed for 3D image analysis, and some of these are directly applicable to studying spatial distribution of pore size in porous media (Lindquist et al., 1996, 2000; Delerue et al., 1999; Delerue and Perrier, 2002; Gladkikh and Bryant, 2007; Glantz and Hilpert, 2007; Ferer et al., 2007; van Dijke and Sorbie, 2007). The use of mathematical morphology has been facilitated further with the inclusion of many of these algorithms in the Image Processing Toolbox available in MATLAB (Mathworks, Natick, MA), thereby opening up a rich suite of techniques that are ideally suitable for study of pore-scale phenomena. Hazlett (1995) and Hilpert and Miller (2001) were among the first to employ this method to simulate pore-scale behavior and to obtain macroscopic hydraulic properties.

Here we present a new algorithm to model the wetting and drying phenomena in soils. This algorithm allows the representation of 3D randomly packed porous media of any geometry (i.e. not restricted to idealized geometries such as spherical or ellipsoidal particles/pore space). The connectivity-, tortuosity-, and hysteresiscausing mechanisms are represented explicitly. Mathematical morphology operations are conducted on pixelized (2D) or voxelized (3D) images either directly taken from mappings of the soil or reconstructed in the computer based on model postulates.

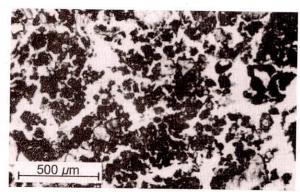
#### SOIL WATER RETENTION CURVE

The WRC of an unconsolidated soil (or any porous medium) depends mainly on the complex topology of the pore space that is governed by the spatial arrangement and distribution of soil particles. Figure 1 shows a thin section of a loam soil that demonstrates the complexity of the pore space. As a result of this complexity, modeling of this relationship can be very challenging even when we consider the medium as a simple capillary system in which surface tension induced by the air—water interface is the only driving force, and ignore other processes such as adsorption and condensation that are known to affect drainage and wetting of soils.

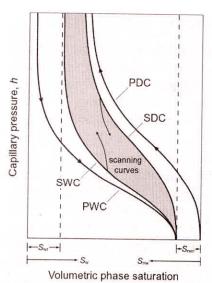
Another complication is that the processes of draining and wetting (imbibition) are dependent on the history of the system. The WRC is a family of characteristic curves that consists of primary and secondary drainage and wetting curves and intermediate scanning curves. Figure 2 shows a schematic of the hysteretic retention curve. Hysteresis of WRC is primarily caused by the effects of pore structure and the hysteresis of contact angle. In addition, the entrapment of air (non-wetting phase) or water (wetting phase)

results in irreducible saturation at the wet or dry end of the retention curve, respectively.

Most of the WRC models used in the fields of soil science and vadose zone hydrology are developed in the form of a mathematical equation that is essentially empirical in nature. Model parameters are obtained by curve-fitting of the observed data. Well-known empirical functions given by Brooks and Corey (1964), van Genuchten (1980), and Russo (1988) are used routinely in many unsaturated flow problems. These functions, while being very useful, lack a physical interpretation of their parameters despite continuing efforts in linking the parameters to various soil properties through regression (Vereecken et al., 1989; Wösten et al., 1999) or artificial neural networks (Schaap and Leij, 1998; Schaap et al., 1998).



**Fig. 1:** Loam soil composed of singly fine grains and grains in clusters, demonstrating the complexity of the pore topology. Adapted from FitzPatrick (1993)



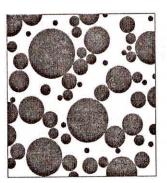
**Fig. 2:** Schematic of the hysteretic retention curves. Adapted from Luckner *et al.* (1989). *S* is the phase saturation and subscript r denotes "residual." PDC, Primary Drainage Curve; SDC, Secondary Drainage Curve; PWC, Primary Wetting Curve; SWC, Secondary Wetting Curve

Another group of WRC models is statistically based, and most models in this group are semiempirical in nature. A mathematical analogy is used between the pore-size distribution and the WRC using the Laplace equation (and therefore it implicitly assumes that the medium behaves as a bundle of capillaries). The pore-size distribution can be arbitrarily assigned as in Kosugi (1994), Or and Tuller (1999), Tuller and Or (2005) and many other studies. Many researchers have taken a step further and tried to establish a functional relationship between soil particle-size distribution (or soil texture) and pore-size distribution (Arya and Paris, 1981; Haverkamp and Parlange, 1986; Assouline et al., 1998; Zhuang et al., 2001). Such relationships can also be derived from fractal concepts as in Tyler and Wheatcraft (1990), Rieu and Sposito (1991), Perrier et al. (1996), and Hunt and Gee (2002). However, these models do not describe how the porous medium can be built from first principle. Consequently, no independent verification of these models is possible, and the empirical relations must be fitted to experimental data without the possibility of revealing any insights into pore-scale processes.

Realizing the need for WRC models with a more sound theoretical footing, Chan and Govindaraju (2003, 2004), CG for short, proposed that one could infer the pore-size distribution from the particle-size distribution on the basis of an assumed arrangement of the soil particles. The idea is that given the particle-size information of a soil, one might assume that the soil particles are arranged in space in a specified random fashion, thus allowing the pore-size distribution be determined. In the development of CG models, two special cases of homogeneous systems of polydisperse spheres were considered: Fully Penetrable Spheres (FPS) and Totally Impenetrable Spheres (TIS). In a FPS system, the spheres are allowed to overlap; thus, the placement of their centers in space follows a Poisson distribution. In the latter (TIS) case, the porous system consists of spheres that are nonoverlapping or impenetrable by each other. Figure 3 shows a 2D rendering of the polydisperse sphere systems. Solid spheres are treated as fundamental building blocks of the porous media. One can compare these idealized systems to the natural soil shown in Figure 1. The overlapping case allows aggregation of spheres as shown, and the resulting medium can be made to represent any arbitrary geometry as closely as desired.

With models of the porous media in place, a difficult problem arises as to how the pore size should be defined. Chan and Govindaraju (2003) argued that the pore throat governs the drainage of fluid through a

porous medium. Therefore, they proposed that a measure of the pore size be the separation distance between the perimeters of two nearest neighboring spheres. In the subsequent study (Chan and Govindaraju, 2004), they adopted the definition of pore size given by Torquato (2002) in which the distance to the surface of a nearest solid sphere from a point picked at random in the void space is considered as the measure of the pore size. With these definitions, analytical equations of the WRC were developed using the Laplace equation to relate the pore sizes to capillary pressures. As an example, Figure 4 shows that the CG–TIS model is in close agreement with the observed data. More details are available in Chan (2005).





**Fig. 3:** Schematic of the polydisperse sphere systems in two dimensions: (*left*) impenetrable hard spheres and (*right*) overlapping spheres. (Chan and Govindaraju, 2004)

It may be noted that among the various models, the CG models allow for a porous medium to be explicitly reconstructed on the computer according to the postulates of a specified particle-size distribution and random spatial arrangement of particles. They are also one of the very few models that allow for construction of the porous medium from more fundamental material properties that are relatively easy to measure (i.e. particle-size distribution rather than pore-size distribution).

Although the CG models were corroborated by the observed soil data in terms of replicating macroscopic soil properties (example in Figure 4), some issues remain unresolved. First, the interconnectivity of the pore space is not specifically accounted for in their models. In fact, the same deficiency exists in all other statistical models. However, the connectedness of the pore space has a significant influence on the WRC. Second, so far all of the models mentioned are primarily used to describe or predict the primary drainage curve. The phenomenon of hysteresis is not considered. To gain better understanding of these issues and perhaps to find ways to improve and extend

the existing theory, numerical pore-scale simulations of the theoretical media are considered next.

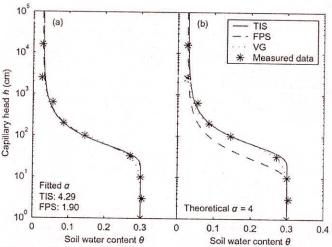


Fig. 4: The measured and estimated primary drainage curves of Beerze podzol II sand (a) with fitted  $\alpha$  (b) with theoretical  $\alpha$ . The variable  $\alpha$  is a scaling parameter described in Chan and Govindaraju (2004). The TIS model provides a very good fit to the measure data. (Chan and Govindaraju, 2004). TIS, totally penetrable spheres model; FPS, fully penetrable spheres model; and VS, van Genuchten model

## PORE-SCALE NUMERICAL MODELING

Understanding multiphase flows in porous media has been motivated by the need to remediate contaminated sites. Most studies have resorted to numerical models of macroscopic flow equations based on a continuum approach (Pinder and Abriola, 1986; Delshad and Pope, 1989). Even though it is recognized that porescale analyses are needed to capture the important geometrical distribution of the different phases, the attention that has been devoted to pore-scale models is relatively small and inadequate (Gvirtzman and Roberts, 1991). It is well known that fluid-fluid and solid-fluid interfacial areas play an important role in a number of processes such as mass transfer, dissolution, and volatilization, as many of these processes are strongly dependant on available surface areas. In addition, more fundamental soil properties, such as drainage and wetting, wettability, capillarity, tortuosity, and connectivity of pores, govern the hydrodynamic behavior of water movement and fate and transport of contaminants in soils. Much of our understanding of these phenomena must come from pore-scale analyses. In fact, the geometry and topology of the pore structure has a strong influence on the constitutive relationships needed for macro-scale continuum models. Thus, pore scale modeling provides us not only with a powerful technique for improving our understanding of fundamental processes governing water and contaminant behavior, but also with a method to estimate fundamental relationships (such as the soil WRC) that are often very difficult and time-consuming to measure experimentally.

One of the primary reasons for inadequate development of pore-scale models is that natural geologic formations have a porous structure that is too complex to represent in complete detail. However, a detailed description is required for meaningful progress into our understanding of processes that operate at the pore scale. One approach is to provide a reasonable idealization of the soil to afford a mathematical analysis, while still incorporating all the relevant characteristics of the medium. Consequently, researchers have pursued improved techniques for representing porous media (see for example Al-Raoush et al., 2003). Several experimental studies have undertaken direct mapping in order to retain the spatial variation in pore structures accurately, of which, imaging techniques and X-ray tomography are examples. Microtomography now allows acquisition of detailed 3D images of porous media at a resolution in the order of 10 µm. However, such experimental studies tend to be expensive.

Macroscopic constitutive relationships, such as the WRC, can be determined through pore-scale modeling. In theory, this task can be attempted from either the Eulerian or Lagrangian perspective. In the Eulerian framework, direct numerical pore-scale simulations using finite-volume or -element techniques can be very challenging and computationally expensive due to the complex morphology of the pore space as well as the difficulty in tracking the wetting phase-non-wetting phase interface. Lattice-Boltzmann technique can better handle the complex morphology and has been used to model pore-scale flow with single phase (Pan et al., 2001) and two phases (Pan et al., 2004; Sukop and Or, 2004). Recently, the method of Smoothed Particle Hydrodynamics (SPH) (a Lagrangian technique) has also shown promise in modeling low Reynolds number flow with complex boundaries (Berry et al., 2004; Morris et al., 1997; Zhu et al., 1999; Tartakovsky and Meakin, 2006). However, the incorporation of surface tension effects in the SPH method has proven to be a formidable obstacle and has met with limited success (Morris, 2000). In addition, methods are computationally expensive, especially in the context of simulating WRC where quasi-static equilibrium is required. Network models simplify the pore space into a network of spherical pores interconnected by cylindrical throats, thereby allowing modeling of pore-scale flow using the Poiseuille equation and the Laplace equation (Blunt,

2001; Hilpert et al., 2003). Pore-network models have shown success in modeling capillary hysteresis (Ioannidis and Chatzis, 1993; Reeves and Celia, 1996; Hilpert et al., 2003; Patzek, 2001; Valvatne and Blunt, 2004). However, calibration of the network models can be problematic because of the difficulty in mapping the porous medium onto the theoretical network using higher order information in the form of multiple point statistics (Okabe and Blunt, 2004). With the ability to include various pore structures for representing features such as the influence of throats with different flow cross sections (triangular) for crevice flows and rough mineral surfaces, pore network models have demonstrated improved capabilities for pore-scale modeling (Iren et al., 1998; Blunt et al., 2002).

Even with a realistic reconstruction of porous media, the problem of inferring macroscopic relationships has remained a numerical challenge in the past. However, with the recent advances in mathematical morphology and the computational power offered by current-day computers, this problem can be addressed to a large degree, and is the subject of this paper. Examples of such methods include medial-axis analysis of pixelized images (Lindquist *et al.*, 1996, 2000; Sok *et al.*, 2002), Delauney tessellation of grain locations (Okabe, 2000), and pore-based morphological operations (Hilpert and Miller, 2001; Gladkikh and Bryant, 2006; Glantz and Hilpert, 2006).

#### **OBJECTIVES**

In light of the literature we have reviewed on porescale modeling (not reproduced here in entirety for brevity), it appears that there is a tradeoff between the computational demand and the ability to account for the complexity of the pore morphology. Although recent pore-network models have shown to provide a computationally efficient way to simulate WRC, the method simplifies the geometry of the pore space, and the network considered is usually of a regular nature so that real soils are not represented very well. The poremorphology-based method holds promise as a better alternative because it fully considers the pore geometry while the computational demand remains manageable. We will extend this method to simulate wetting and intermediate scanning curves. In this process, we develop a new tool for understanding the processes of drainage and wetting of soils with different texture and structure. The specific objectives are:

 Generalization of the pore-morphology-based simulation technique. We extend the poremorphology-based technique to model the wetting process

- as well. Certain mechanisms of hysteresis, such as the ink-bottle effect and the entrapment of wetting and non-wetting phases, will be incorporated.
- Investigation of effects of hysteretic mechanisms on WRC. We will include some of the mechanisms contributing to hysteresis into our simulation algorithm.

# ALGORITHM FOR PORE-MORPHOLOGY-BASED SIMULATIONS AND PROPOSED EXTENSION

Following the notation and methodology of Hilpert and Miller (2001), a novel approach to simulate drainage of a porous medium using basic morphological operations is briefly presented here. Two fundamental concepts in mathematical morphology are used in this method: erosion and dilation. The morphological erosion E of a set E by a structuring element E is the locus of the centers E of E of E that are included in E,

$$E_s(S) = \begin{Bmatrix} r : S_r^r \subset X \end{Bmatrix} \dots (1)$$

The subscript r = r denotes the translate of S by the vector r = r. Equation (1) can also be written as,

$$E_s(S) = X \$ \S \qquad \dots (2)$$

Where \$ stands for the Minkowski subtraction and S for the reflected set of S with respect to the origin,  $S = \left\{-\frac{r}{r} : \frac{r}{r} \in S\right\}$ . For a symmetric structure element, S = S. The dilation D of S by S is the locus of the centers of  $S_r$  that intersect (or touch) S,

$$D_s(X) = \begin{Bmatrix} r : S_r^r \cap X \neq \emptyset \end{Bmatrix} \qquad \dots (3)$$

Similar to erosion, (3) can be written as,

$$D_s(X) = X \oplus \ \ \ \ \ \ \dots \ (4)$$

where  $\oplus$  stands for the Minkowski addition. These two basic morphological operations can be combined to form new operations such as an opening (an erosion followed by a dilation) that is the heart of this poremorphology-based method. The morphological opening O of X is defined as,

$$O_s(X) = (X \$ \S) \oplus S \qquad \dots (5)$$

#### Methodology

Consider a porous medium with the top connected to a Non-Wetting Phase (NWP) reservoir and the bottom connected to a Wetting Phase (WP) reservoir (see Figure 5). This is typical of a suction or pressure cell experiment to measure WRC. The following procedure is given by Hilpert and Miller (2001) to simulate the drainage curve.

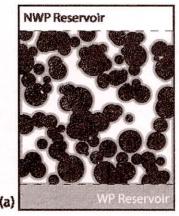
- 1. The porous medium, including the pore space, is first discretized into voxels that can be represented digitally. Note that the resolution of this discretization will affect the accuracy of the results.
- 2. Initially the medium is saturated with the WP. The capillary pressure *h* is zero. The NWP only exists in the top reservoir.
- 3. The pore space P is eroded by a spherical structuring element S of diameter D. The corresponding capillary pressure is calculated using  $h=4\sigma/D$  where  $\sigma$  is the interfacial tension. Since the capillary pressure is inversely related to the diameter, a large diameter is initially used and is then decreased incrementally. Note that the structuring element is also discretized with the resolution as the porous medium.
- 4. The portion of the eroded pore space connected to the NWP reservoir is identified through a connectivity analysis (with 4- or 6-connected neighborhood for 2D or 3D problem, respectively). A morphological dilation is performed on this portion with the same structuring element *S(D)*
- 5. The NWP effective saturation  $S_{nw}$  is calculated as a volume ratio of the dilated pore space to the entire pore space.
- 6. Repeat step (3)–(5) with a smaller D until the entire retention curve is obtained.

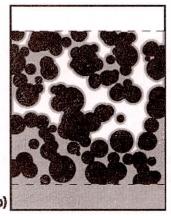
In terms of mathematical morphology, the NWP saturation is given as,

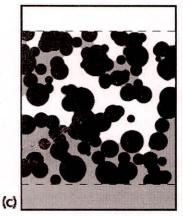
$$S_{mv}(D) = \frac{\operatorname{Vol}\left\{C\left[P\$\$(D)\right] \oplus S(D)\right\}}{\operatorname{Vol}(P)} \qquad \dots (6)$$

where C represents the identification of eroded pore space that is connected to the NWP reservoir. The WP saturation is simply given by  $S_w(D) = 1 - S_{nw}(D)$ . Figure 5 demonstrates graphically the essential part of the simulation procedure in 2D. The described approach assumes that the contact angle is zero and that a thin film of the WP exists and is connected to the WP reservoir at all times. The volume of WP contributed by this thin film is ignored. Hilpert and Miller (2001) has shown that this approach is more efficient than conventional techniques, such as finite-element and lattice-Boltzmann, since only a predetermined number of computational steps is required on logical variables that allow efficient use of memory.

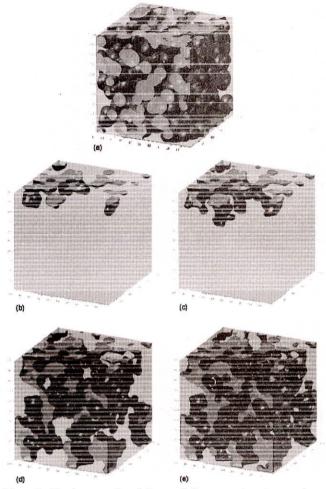
An example of the drainage simulation was performed using a FPS medium (generated in accordance with Chan and Govindaraju, 2004) with a lognormal particle-size distribution. The simulation results are visualized in Figure 6. This figure reveals that the method we propose is not restricted to regular geometries. The drained NWP pore space is shown. As capillary pressure increases, more pore space is emptied. One can observe that the connectivity of pore space plays a significant role in the drainage of the porous medium.







**Fig. 5:** Illustrations of the pore-morphology-based drainage simulation in 2D: (a) the pore space P is eroded by a circular structuring element S; (b) the eroded pore space connecting to the NWP reservoir is selected; (c) the selected portion is dilated to recover the NWP invaded pore space. (After Hilpert and Miller, 2001)



**Fig. 6:** Drainage simulation of the overlapping sphere medium. (a) A simulated medium 100<sup>3</sup> voxels in size with the solid phase being visualized. (b)–(e) The NWP invaded pore space is visualized. Capillary pressure increases gradually from (b) to (e)

#### **Extension to Drainage Algorithm**

In the existing drainage algorithm, the initial pore space is always assumed to be entirely filled with the WP. The use of such initial condition is valid for the primary drainage curve. However, in order to simulate the drying scanning curves, one must be able to specify the existing condition of the pore space and this condition must be taken into account when finding a new equilibrium with an incrementally smaller S(D). Different entrapment strategies should also be considered. Currently, no WP trapping is explicitly considered; "isolated" pockets of WP remain at the corner and recesses of the pore space and their volume continues to decrease as capillary pressure increases. Options can be provided in the proposed algorithm to either completely drain these isolated WP pockets or preserve their volume throughout the simulation of the entire drainage curve. We achieve these extensions on

the drainage algorithm through a combination of set operations and connectivity analysis.

#### **Wetting Simulations**

The current drainage algorithm can be characterized by a three-step process: erosion—connectivity analysis—dilation. A reshuffling of this three-step process is required for a wetting simulation. We are able to demonstrate the "ink-bottle" phenomenon given the proposed wetting algorithm. NWP entrapment is considered as well. It should be noted that by combining the wetting and drainage algorithms with the consideration of a given existing condition (NWP distribution in the pore space), the simulations of scanning curves with hysteresis loops are made possible. The complete WRC can be obtained as a result.

#### COMPUTATION OF INTERFACIAL AREA

Since the pore-morphology-based method fully considers the pore geometry, the simulation results can be used to investigate the role of interfacial area in the constitutive relationship of capillary pressure and saturation. An accurate method of estimating the interfacial area from the simulation results is therefore required to accomplish this goal. Dalla et al. (2002) used the marching-cube algorithm (Lorensen and Cline, 1987) to approximate the interfacial surfaces between WP, NWP, Solid Phase (SP). Area estimates using this method, however, are not accurate even with high resolution. In this study, we adopt a voxel-based approach (Mullikin and Verbeek, 1993; Windreich et al. 2003) to estimate surface area. This voxel-based surface area estimation is a natural extension of the 2D perimeter estimation theory. Similar to perimeter estimation, where different combination of pixels account for different lengths of the perimeter, in the voxel-based surface area estimation, the surface voxels are classified into different classes, with a weighted value of the surface area assigned to each class. The total surface area of a 3D digitized object is simply a linear combination of these weights,

$$\hat{S} = \sum_{i=1}^{9} W_i N_i \qquad \dots (7)$$

where  $N_i$  is the number of surface voxels belonging to a class member i, and  $W_i$  is the corresponding weight. Details of this method are provided in Chan (2005). Results of this procedure are presented for an example case in Figure 7, where the porous media was constructed according to the postulates of Chan and Govindaraju (2003, 2004). Figure 7 shows that the

relationship between saturation, water pressure and interfacial area is not a simple one that can be easily collapsed into a single unique curve.

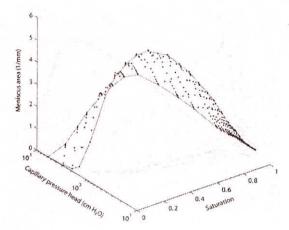


Fig. 7: Meniscus area per unit volume as a function of capillary pressure and saturation. The blue color indicates drainage, while the red color indicates wetting

#### **EXAMINATION OF HYSTERESIS**

The proposed algorithm allows a relatively efficient way, as opposed to expensive and timeconsuming experiments, to investigate hysteresis manifested in the WRC. With our proposed technique, we simulated the primary drainage and wetting curves, along with several scanning curves for a soil generated on the computer according to Chan and Govindaraju (2003, 2004) procedure. Figure 8 shows the WRC with the primary wetting and drying curves, along with several scanning curves as conceptualized in Figure 2. The figure shows that the modified algorithm presented in this paper is able to model hysteretic behavior (see also Figure 7 for scanning curves).

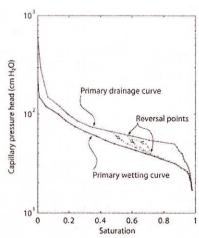


Fig. 8: Illustration of primary drainage and wetting curves along with some scanning curves as computed using the drainage-wetting simulation algorithm

#### LIMITATIONS AND CONCLUSIONS

This paper summarizes the use of mathematical morphology for determining water retention curve from digitized or computer-generated images of porous media. The method presented here is able to account for the complex pore geometry and compute hysteretic relationships and interfacial areas-both of which are fundamental to understanding fluid behavior soils.

It is not immediately clear to us at this stage as to how the hysteresis of contact angles can be incorporated. The use of an oblate spheroid can be considered. However, the hysteresis in the advancing and receding contact angles is a dynamic process. The poremorphology-based method performs a quasi-steady state simulation, and as such this limitation might hinder the incorporation of the contact angle hysteresis.

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