Pore-morphology-based simulations of drainage and wetting processes in porous media

T. P. Chan and Rao S. Govindaraju

ABSTRACT

Soil hydraulic properties relating saturation, water pressure, and hydraulic conductivity are known to exhibit hysteresis. 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. We develop 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 in both drainage and wetting processes, and their role in determining macroscopic fluid behavior is made explicit. Using this method, we present simulation results that demonstrate hysteretic behavior of wetting and non-wetting phases during both drainage and wetting cycles. A new method for computing interfacial surface areas is developed. The pore-morphology-based method is critically evaluated for accuracy, sample size effects, and resolution effects. It is found that the method computes interfacial areas more accurately than existing methods and allows for (i) examination of relationships between water pressure, saturation and interfacial area for hysteretic soils, and (ii) comparisons with previously developed theoretical models of soil hydraulic properties. The pore-morphology-based method shows promise for applications in vadose zone hydrology.

Key words | hysteresis, mathematical morphology, retention curve, unsaturated flow

INTRODUCTION

Understanding multi-phase flow in porous media has largely 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 (Delshad & Pope 1989; Pinder & Abriola 1986). Even though it is recognized that pore-scale analyses are needed to capture the important geometrical distribution of the different phases, the attention that has been devoted to pore-scale models has been relatively small and inadequate (Gvirtzman & 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. In addition, tortuosity and connectivity of pores govern the hydrodynamic behavior of water movement and fate and transport of contaminants in soils. The geometry and topology of the pore structure have a strong influence on the constitutive relationships needed for macro-scale continuum models. Pore-scale modeling is needed not only for improving our understanding of fundamental processes governing water and contaminant behavior, but also to estimate fundamental relationships (such as the soil water retention curve) that otherwise have to be obtained from difficult and time-consuming experiments.

Macroscopic constitutive relationships, such as the water retention curve (WRC), can be determined from either
the Eulerian or Lagrangian perspectives. 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 interface between the wetting and non-wetting phase. The 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 & Or 2004). Smoothed particle hydrodynamics (a Lagrangian technique) has also shown promise in modeling low Reynolds number flow with complex boundaries (Morris et al. 1997; Zhu et al. 1999; Berry et al. 2004). However, the incorporation of surface tension effects has proven to be a formidable obstacle and has met with very limited success (Morris 2000). It is believed that other Lagrangian methods will suffer from similar limitations. In addition, these methods are computationally expensive, especially in the context of simulating WRC where quasi-static equilibrium is required.

The water retention curve, due to its hysteretic nature, is not a single unique relationship, but a family of characteristic curves that consists of primary and secondary drainage and wetting curves as well as intermediate scanning curves. Hysteresis of WRC is primarily caused by the effects of pore structure and the hysteresis of contact angle. Other factors, such as wetting phase (WP) and non-wetting phase (NWP), entrapment, and ink-bottle effect, also contribute to hysteresis.

Pore-network models have shown success in modeling capillary hysteresis (Ioannidis & Chatzis 1993; Reeves & Celia 1996; Blunt 2001; Hilpert et al. 2005; Valvatne & Blunt 2004). However, their calibration can be problematic because of the difficulty in mapping the porous medium onto the theoretical network. Even with a realistic reconstruction of porous media, the problem of inferring macroscopic relationships has remained a numerical challenge in the past. With recent advances in mathematical morphology and the computational power offered by current-day computers, this problem can be addressed and is the subject of this study. Examples of such methods include medial-axis analysis of pixelized images (Lindquist et al. 1996, 2000), Delauney tessellation of grain locations (Okabe 2000), and pore-based morphological operations (Hilpert & Miller 2001).

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 have been developed for 3D image analysis, and some of these are directly applicable to studying spatial distribution of pore sizes in porous media (Lindquist et al. 1996, 2000; Delerue et al. 1999, Delerue & Perrier 2002; Ferer et al. 2007; Gladikh & Bryant 2007; Glantz & Hilpert 2007; van Dijke & Sorbie 2007). Hazlett (1995) and Hilpert & Miller (2001) were among the first to employ this method to simulate pore-scale behavior and obtain macroscopic hydraulic properties.

In this work, the pore-morphology-based method is extended to incorporate both drying and wetting processes and subsequently hysteresis as well. An improved method of estimating interfacial areas is also presented to explore the relationship between capillary pressure, saturation, and interfacial area. This is followed by a critical evaluation of the capabilities of the new algorithms for simple geometries and for modeled soils. The proposed simulation technique is then used to investigate the validity of the fully penetrable spheres (FPS) model developed by Chan & Govindaraju (2004). Finally, important conclusions highlighting the strengths and limitations of this work are presented.

PORE-MORPHOLOGY-BASED DRAINAGE SIMULATIONS

The pore-morphology-based method uses mathematical morphology to perform a series of operations on the pore space of a porous medium to simulate the drainage and invasion of a wetting fluid, such as water. This technique is analogous to using a sphere of a given size to probe through the pore system (Chan & Govindaraju 2005). The volume of the pore system accessible to the sphere is presumed drained, and the size of the sphere determines the capillary pressure (suction) applied to drain the medium. By using successively smaller diameter spheres, a complete drainage curve can be obtained (Chan & Govindaraju 2006).
Following the notation and methodology of Hilpert & Miller (2001), a novel approach to simulate drainage of a porous medium using basic morphological operations is presented here briefly. Two fundamental concepts in mathematical morphology are used in this method: erosion and dilation. The morphological erosion $\varepsilon$ of a set $X$ by a structuring element $S$ is the locus of the centers $\vec{r}$ of the $S_{\vec{r}}$ that are included in $X$:

$$
\varepsilon_S(X) = \{ \vec{r} : S_{\vec{r}} \subset X \} = X \ominus \hat{S}
$$

(1)

where $\ominus$ stands for Minkowski subtraction and $\hat{S}$ for the reflected set of $S$ with respect to the origin, $\hat{S} = \{ -\vec{r} : \vec{r} \in S \}$. The subscript $\vec{r}$ denotes the translate of $S$ by the vector $\vec{r}$. For a symmetric structure element, $\hat{S} = S$. The dilation $\mathcal{D}$ of $X$ by $S$ is the locus of the centers of the $S_{\vec{r}}$ that intersect (or touch) $X$:

$$
\mathcal{D}_S(X) = \{ \vec{r} : S_{\vec{r}} \cap X \neq \emptyset \} = X \oplus S
$$

(2)

where $\oplus$ stands for Minkowski addition. These two basic morphological operations can be combined in different orders to form new operations. For example, the definition of a morphological opening $\mathcal{O}$ of $X$ is an erosion followed by a dilation:

$$
\mathcal{O}_S(X) = (X \ominus \hat{S}) \oplus S
$$

(3)

These operations play a central role in the simulation of drainage of porous media. In order to perform these operations on the pore space of a medium, the porous medium has to be digitized/discretized such that the pore space is represented by voxels (unit cubes, analogous to pixels in 2D) on a cubic lattice. The structuring element used is a digital sphere in 3D (or a disk in 2D). One way to define a digital sphere of integer diameter $D$, given by Hilpert & Miller (2001), is

$$
S(D) = \{ \vec{r} \in \mathbb{Z}^3 : (\vec{r} - \vec{c})^2 \leq D^2/4 \}
$$

(4)

where the center of the sphere is $c_i = D/2 + 1/2$ for each dimension $i = 1, 2, 3$, and $\mathbb{Z}^3$ is the underlying discrete space for the cubic lattice.

### METHODOLOGY OF DRAINAGE SIMULATIONS

We 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. This is typical of a suction or pressure cell experiment to measure water retention curve. The following procedure is adapted from Hilpert & Miller (2001) to simulate the drainage curve:

1. The porous medium is first discretized into voxels for digital representation.
2. Initially the medium is saturated with the WP. The capillary pressure $h$ is zero. NWP only exists in the bottom reservoir.
3. The pore space $P$ is eroded by a spherical structuring element $S$ of diameter $D$:

$$
P_e(D) = P \ominus S(D)
$$

(5)

where the subscript $e$ signifies that the pore space has been eroded. The corresponding capillary pressure is calculated using the Laplace equation: $p = 4\sigma/D$ where $\sigma$ is the interfacial tension. Since the capillary pressure is inversely related to the diameter, a large diameter is initially used, and is decreased incrementally. The structuring element is also discretized with the same resolution as the porous medium.

4. The portion of the eroded pore space connected to the NWP reservoir ($P_{ce}$) is identified:

$$
P_{ce}(D) = C^n|P_e(D)|
$$

(6)

where $C$ represents the connectivity analysis using a 3D six-connected neighborhood. The superscript $n$ indicates the connectivity to the NWP reservoir. The connectivity analysis is accomplished by labeling all the connected components in the eroded pore space and then finding the components with a label that corresponds to that of the NWP reservoir.

5. A morphological dilation is then performed on this connected portion using the same structuring element $S(D)$ as in the erosion process in Step (3). The result of this dilation is the NWP-occupied pore space.

$$
P_n(D) = P_{ce}(D) \oplus S(D)
$$

(7)

6. The NWP effective saturation $\Theta_n$ is calculated as a volume ratio of the dilated pore space and the entire pore space:

$$
\Theta_n(D) = \frac{\text{Vol}[P_n(D)]}{\text{Vol}[P]}
$$

(8)
Vol\[\cdot\] represents the determination of volume by counting the “on” voxels. The WP saturation is simply given by

\[
\Theta_w(D) = 1 - \Theta_n(D)
\]

(9)

Steps (3)–(6) are repeated with an incrementally smaller diameter, \(D_{\text{new}} = D - 1\), until the entire retention curve is obtained.

The WP saturation should decrease monotonically as \(D\) decreases. The use of digital sphere as a structuring element (as in (4)), however, does not guarantee the monotonicity of \(\Theta_w(D)\) because the shape of the digital sphere is not self-similar nor is it convex. Hilpert & Miller (2001) recognized this and suggested that a modified version of the spherical structuring element should be used instead of (4) to alleviate this situation:

\[
S'(1) = S(1); \quad S'(n) = S(n) \cup S(n - 1)
\]

(10)

where \(n = 2, 3, 4, \ldots\). This approach assumes that the contact angle is zero. It also assumes that thin films of the WP exist, coating the solid phase in all drained pore space, such that the entire WP is connected to the WP reservoir at all times. The volume of the WP contributed by the thin films is, however, ignored. The results of drainage simulation using the pore morphology-based method have been validated by experimental data in Hilpert & Miller (2001).

The method has also been shown to be more efficient than conventional techniques, such as finite-element and lattice Boltzmann, since only a predetermined number of computational steps is required. Logical (1-byte) variables are used to store the digitized medium, thus allowing efficient use of memory. The algorithm can also take advantage of parallel computing.

**EXTENSIONS TO THE EXISTING METHODOLOGY**

The existing pore-morphology-based method treats the porous medium as a simple capillary system where the equilibrium state between the capillary pressure and the curvature of the NWP–WP interface is governed by the Laplace equation. The radius of the structuring element is also the radius of the curvature of all NWP–WP interfaces that exist within the medium. The remaining pore space, which is not accessible by the probe and not connected to the NWP reservoir, is WP saturated, and the WP saturation is determined as a ratio of the WP-saturated pore volume to the total pore volume.

Thinking along similar lines, this work aims to extend this current methodology in several ways:

- To allow the option during drainage that any disconnected WP is drained;
- To allow the option of WP entrapment during drainage (all disconnected WP are therefore not drained);
- To simulate wetting of a porous medium with no NWP trapping;
- To simulate wetting with consideration of NWP entrapment;
- To allow simulation of wetting and drying scanning curves.

The following sections explain the algorithms developed to accomplish these tasks.

**Drainage simulations**

In the existing drainage algorithm, the pore space is initially assumed to be filled entirely with the WP, i.e. the initial (or existing) condition is one of an empty NWP-filled pore space: \(P_{n,ex} = \{0\}\). The use of this initial condition is valid for the primary drainage curve. However, in order to simulate the drying scanning curves, one must be able to specify an existing state of the pore space as an initial condition and find a new equilibrium with an incrementally smaller \(S(D)\).

The following step should be added immediately after Step (5) of the existing drainage procedure to allow for construction of drying scanning curves:

(i) The NWP-filled pore space obtained in Step (5) is combined with the existing NWP-filled pore space:

\[
P_{n,1}(D) = P_n(D) \cup P_{n,ex}(D)
\]

(11)

Typically \(P_{n,ex}(D)\) is the NWP-filled pore space obtained from the previous simulated state such that \(P_{n,ex}(D) = P_{n,1}(D + 1)\). Subsequently, \(P_{n,1}(D)\) replaces \(P_n(D)\) and becomes the default (Type I) solution of the drainage simulation. Although no WP trapping is explicitly
considered here, “isolated” pockets of WP remain at the corners and recesses of the pore space, and their volume continues to decrease as capillary pressure increases (i.e. with structuring elements of smaller diameters). These isolated pockets continue to drain because it is assumed that a thin film of WP coating the entire solid phase connects these pockets to the WP reservoir.

One slight inconsistency in the current scheme, as noted by Hilpert & Miller (2003), is that if a pore throat is invaded by the NWP simultaneously from two sides, the pore throat cannot be completely drained and a WP ring is left in the throat. Two special cases can be considered in light of this. The first case is to have all the disconnected WP (from the WP reservoir) drained. To implement this, the following steps may be inserted immediately following Step (i):

(ii) The WP-occupied pore space is found by an exclusive OR (XOR) operation:

$$P_w(D) = XOR[P_n,1(D), P]$$

$$= [P_n,1(D) \cup P] \cap [P_n,1(D) \cap P]^C$$  \hspace{1cm} (12)

(iii) The portion of the WP-filled pore space connected to the WP reservoir, \(P_{cw}(D)\), is identified through a connectivity analysis: \(P_{cw}(D) = Cw[P_w(D)]\).

(iv) The NWP-filled pore space without disconnected pockets of WP can then be obtained by an XOR operation:

$$P_{n,2}(D) = XOR[P_{cw}(D), P].$$

Thus, \(P_{n,2}\) becomes the solution of Type II drainage simulation where all disconnected pockets of WP are drained.

Another option (the second case) is to allow WP entrapment during drainage. In other words, once a pocket of WP is disconnected with the WP reservoir, it will not be drained and its volume remains unchanged for the rest of the drainage simulation. This option is perhaps useful when the porous medium is not strongly wet. To implement this option, the following steps may be inserted after Step (i):

(ii) The existing WP-filled pore space is identified:

$$P_{w,ex}(D) = XOR[P_{n,ex}(D), P].$$

(iii) A connected component analysis is performed on \(P_{w,ex}(D)\) to find the portion of the existing WP-filled pore space that is connected to the WP reservoir.

The disconnected or isolated pockets of WP, \(P_{dcw}\), are then found by

$$P_{dcw}(D) = XOR[Cw[P_{w,ex}(D)], P_{w,ex}(D)]$$  \hspace{1cm} (13)

(iv) The NWP-filled pore space with trapped WP can then be obtained by

$$P_{n,3}(D) = XOR[P_{dcw}(D), P_{n,1}(D)] \cap P_{n,1}(D)$$  \hspace{1cm} (14)

\(P_{n,3}\) becomes the solution of the Type III drainage simulation with the third option where disconnected WP is considered trapped.

The existing drainage algorithm has been extended to consider two other cases of with and without WP entrapment. But more importantly, the extended algorithm can now accommodate any initial state of the pore space and simulate drying and wetting processes. The hysteretic nature of the retention curve can now be modeled and simulated with further extension of the algorithm as described below.

**Wetting simulations**

The proposed wetting algorithm is largely inspired by the ink-bottle effect. However, due to the use of a spherical structuring element, the contact angle is always assumed to be zero. Thus, the hysteresis due to differences in advancing and receding contact angles is not captured by this proposed algorithm. The wetting algorithm involves the following steps:

1. A morphological opening is first performed on the pore space:

$$P_o(D) = S(D) \cap P = [P \ominus S(D)] \ominus S(D)$$  \hspace{1cm} (15)

If NWP entrapment is considered, then disconnected pockets of NWP that are present in the existing condition have to be added to the opened pore space, such that

$$P_o(D) = XOR[Cw[P_{n,ex}(D)], P_{n,ex}(D)] \cup OS(D)$$  \hspace{1cm} (16)

2. The potential WP-filled pore space is found by

$$P_w(D) = XOR[P_o(D), P].$$ Not all of this pore space will
eventually be filled by the WP. A connectivity analysis in the next step will determine to what extent this potential pore space is to be filled.

(3) The WP-filled pore space is found by locating the portion of $\tilde{P}_w(D)$ that is connected to WP reservoir:

$$P_w(D) = C^w[\tilde{P}_w(D)]$$

(17)

(4) Finally, the NWP-filled pore space is found by considering both the WP-filled pore space and the existing NWP-filled pore space:

$$P_n(D) = \text{XOR}[P_w(D), P_{n,ex}(D)] \cap P_{n,ex}(D)$$

(18)

The NWP and WP saturations can be obtained via (8) and (9), respectively.

Figure 1 illustrates the wetting algorithm on a 2D porous medium. The major difference between the proposed algorithm and that of Hilpert & Miller (2001) lies in the order of the connectivity analysis and the dilation. In the drainage procedure, the erosion is followed by a connectivity analysis to the NWP reservoir, then by a dilation; whereas in the wetting procedure, the erosion is followed immediately by a dilation, which combines as a morphological opening (Figure 1(a, b)). The connectivity analysis to the WP reservoir is carried out as the last step (Figure 1(c)).

The entire wetting curve can be simulated if an incrementally larger $D$ is used. The existing condition of the pore space is usually specified as $P_{n,ex} = P_n(D-1)$. However, to simulate the primary wetting curve without NWP entrapment, the initial condition is always a fully NWP-filled pore space such that $P_{n,ex} = P$. In fact any single point on the primary wetting curve can be obtained independently from the simulator regardless of order because the initial condition is always the same. The same argument also holds true for the simulation of primary drainage curve as well if the default option is used (where no explicit WP entrapment is considered).

### Simulations of scanning curves

The simulation of scanning curves is now possible when the drainage and wetting algorithms are used in appropriate sequences, and the existing condition of the pore space is specified using the previous simulated state. For example, to simulate a wetting scanning curve one can use the following procedure:

(1) Start with a point on the primary drainage curve, given by a drainage simulation using a structuring element of diameter $D$ with initial condition $P_{n,ex} = [0]$.  
(2) The NWP-filled pore space obtained from the previous step is used as the existing condition in a wetting simulation with structuring element of diameter $D + 1$.  
(3) Repeat Step (2) with an incrementally larger diameter.

At any point in the above procedure, one can reverse the wetting and continue with a drainage simulation with a smaller $D$, and the hysteresis loop can be obtained.

### COMPUTATION OF INTERFACIAL AREA

Traditionally, Darcy’s law has been extended to describe the macroscopic flows of two or more immiscible fluids in a...
porous medium. The WRC (capillary pressure–saturation relationship) and the relative hydraulic conduction function (hydraulic conduction–saturation relationship) are needed in this continuum approach. However, these constitutive relationships, combining with Darcy’s empirical flow equation, often fail to describe hysteresis effects where, for a given capillary pressure, many distributions of the fluid phase are possible within the porous medium, resulting in many possible values of saturation (Gray & Hassanizadeh 1991). Realizing the importance of thermodynamics and geometry of fluid–fluid and fluid–solid interfaces, researchers have developed new theories for multi-phase flows that incorporate the specific interfacial area, area per unit volume of the porous medium, as a key variable in the formulation of flow equations (Gray & Hassanizadeh 1998; Gray 1999; Gray & Miller 2005; Miller & Gray 2005). In particular, it is proposed that the specific interfacial area be included as a new variable in the constitutive relationship of capillary pressure and saturation (Hassanizadeh & Gray 1990, 1993a, b). The interfacial area can be expressed as a function of capillary pressure and saturation, thereby creating a 3D surface.

The existence of a relationship between capillary pressure, saturation, and interfacial area has gained considerable support from both experiments and numerical modeling. Cheng et al. (2004) studied drainage and imbibition of artificial random porous media by experimenting on “micro-models” that were fabricated using photo-sensitive polymer and glass slides. They have shown from experimental results that the capillary pressure, saturation, and interfacial area form a unique and invertible surface for the 2D random porous medium that they used in their work. They have also demonstrated experimentally that hysteresis can be a result of changes in capillary-dominated interfaces. Pore-network models (Reeves & Celia 1996) have also been used to demonstrate the existence of such a functional relationship between the three variables. Gvirtzman & Roberts (1991) derived interfacial area as a function of capillary pressure and saturation from cubic and rhombohedral packings of identical spheres.

Dalla et al. (2002) presented a method for calculating interfacial areas based on the results from Hilpert & Miller’s (2003) pore morphology-based drainage simulator. They used the marching-cube algorithm (Lorensen & Cline 1987) to approximate the interface with triangulated surfaces. By summing the triangles of the iso-surface, they were able to estimate surface areas of the meniscus (NWP–WP) interface, the NWP, the WP, as well as the solid phase (SP) (see Figure 2). However, the iso-surface generated by the marching-cube algorithm is often not able to accurately represent the true surface of the interface, even under high resolution (Dalla et al. 2002). Also, the estimated surface area fails to converge to the true surface area with increasing resolution and increasing area (Kenmochi & Klette 2000).

**VOXEL-BASED SURFACE AREA ESTIMATOR**

The estimation of surface area from a digitally represented object (in the form of voxels) is a challenging problem (Windreich et al. 2003). An immediate concern is that a digital representation is merely an approximation of the true object with accuracy strongly dependent on the degree of resolution. The voxels present on the surface of the object form a jagged outline as opposed to the continuous true surface. If one were to just count the number of surface voxels, the estimated surface area would have been grossly overestimated. In addition, for the same digital surface, more than one continuous surface of different areas can be represented, resulting in problems of non-uniqueness. The voxel-based technique, first presented by Mullikin & Verbeek (1993) and further extended by Windreich et al. (2003), has been shown to provide a fast and accurate scheme to evaluate surface area of a digitized object. We present a modified algorithm to calculate the interfacial surface area from the results generated by the pore-morphology-based drainage–wetting simulator.
The voxel-based surface area estimation is a natural extension of the 2D perimeter estimation theory (Mullikin & Verbeek 1993). In the voxel-based estimation of surface area, the surface voxels are classified into different classes, with a weighted value of the surface area assigned to each class. To compute the total surface area $S$ of an object, a linear combination of these weights is used:

$$S = \sum_{i=1}^{9} W_i N_i$$

where $N_i$ is the number of surface voxels belonging to a class member $i$ and $W_i$ is the corresponding weight. A surface voxel is defined as a voxel that is 6-connected to the background.

Despite what initially appears to be a large number of combinations, upon rotation and mirroring, only nine classes of surface voxels are possible. Figure 3 shows these nine unique classes, $S_{1-9}$ with the darker voxel being the subject surface voxel of concern, and the lighter voxels its neighbors. Since $S_{1-3}$ can only be found on a planar surface, Mullikin & Verbeek (1993) estimated the weights for surface voxel classes $S_{1-3}$ by minimizing the mean square error for random plane orientation. They found that $W_1 = 0.894$, $W_2 = 1.3409$, and $W_3 = 1.5879$. The coefficient of variation ($CV = \sigma/\mu$) is quite small at 2.33%. For voxel classes $S_{4-6}$ that occur on a curved surface, they used the spatial grid method (Hahn & Sandau 1989) to obtain the weights for these voxels as $W_4 = 2$, $W_5 = 8/3$, and $W_6 = 10/3$. Windreich et al. (2003) assigned the rest of the weights for voxel classes $S_{7-9}$ as $W_7 = 1.79$, $W_8 = 2.68$, and $W_9 = 4.08$. The occurrence of $S_{4-9}$ is quite rare compared to the first three types. The estimated surface area should not be very sensitive to the weights selected for these voxel classes. To achieve a better accuracy and to eliminate a certain bias relating to the size of the surface, both the foreground and background surface voxels should be considered. The estimated surface area of an object is the average of the foreground and background surface areas.

**SIMULATION OF RANDOM POROUS MEDIUM**

One of the objectives of this study is to test the theories developed in Chan & Govindaraju (2003, 2004). The pore-morphology-based method can simulate the drainage curve for a given proposed theoretical porous media, and the simulated drainage curve can be compared to the proposed water retention models. Theoretical porous media generated by the Random Cluster (RC) model and the Fully Penetrable Spheres (FPS) model are considered in this study.

For systems of overlapping spheres, the simulation procedure is as follows. For a uniform particle-size distribution ($d_{max} = \text{maximum particle size, } \phi = \text{porosity}$) specified by the RC model, the number of spheres per unit volume $\rho_s$ is given as

$$\rho_s = \frac{24\ln(\phi)}{\pi d_{max}^3}$$

whereas for a lognormal particle-size distribution in the FPS model $\rho_s$ is

$$\rho_s = \frac{3\ln(\phi)}{4\pi m_3}$$

where $m_3$ is the third moment of the log-transformed particle diameter (see (24)). To generate a realization of the medium of known porosity and particle-size parameters,
a random location is picked within a unit volume and a sphere with a diameter drawn from a given distribution (uniform for RC model; lognormal for FPS model) is placed at that location. Placing of spheres continues until the number of spheres reaches the value of $\rho_y$. Discretization of the simulated medium is done according to the specified resolution. The center of a spherical structuring element as in (4) and (10) does not always lie squarely on the discrete space $Z^3$. For even-diameter spheres, the centers are located at subsets of $Z^3 \cap \{(1/2, 1/2, 1/2)\}$. To apply a morphological operation, the center of the structuring element is taken to be $c_i$ and $c_i = \pm 1/2$ for even and odd diameters, respectively.

**IMPLEMENTATION**

Algorithms discussed in previous sections are all implemented in MATLAB – a high-level computer language with interactive interface developed by The MathWorks (Natick, MA). The details of the implementation of these morphological functions are available in the Image Processing Toolbox User’s Guide (The MathWorks 2005).

The function to estimate interfacial surface area was linked to MATLAB through a MEX-file interface. The function utilizes the neighborhood block processing module available in the Image Processing Toolbox. The neighborhood module provides sequential access to each voxel of the digitized pore space and its neighborhood voxels. To estimate the surface area of, say, the NWP–WP meniscus interface, each voxel in the NWP-filled pore space ($P_n$) is checked for connectivity (6-connectedness) to the background, i.e. the WP-filled pore space ($P_w$). If the voxel is identified as a surface voxel, then it is classified into one of the nine surface voxel classes by checking the spatial arrangement of its six face-connected neighbors according to Figure 3. The surface area is the cumulative sum obtained via (19). The same procedure needs to be repeated using $P_w$ as foreground and $P_n$ as background. Finally, the NWP–WP meniscus area, $a_{aw}$, is calculated as the average of the two surface areas. The surface areas for the NWP, WP, and SP (Figure 2) can be obtained in a similar fashion.

The programming routine to generate realizations of the overlapping sphere medium was linked to MATLAB directly. The program takes the porosity $\phi$ and the particle-size parameters ($d_{max}$ in the RC model; $\mu_y$ and $\sigma_y$ in the FPS model), and generates a digital porous medium with the desired sample size and resolution.

**DRAINAGE–WETTING SIMULATION RESULTS**

**Simple pore geometry results**

The pore-morphology-based approach for drainage simulation has been previously tested and compared with experimental data by Hilpert & Miller (2001) and Dalla et al. (2002). Several pore structures with simple geometries were considered to test the proposed drainage–wetting algorithms (Chan 2005). For brevity, the efficacy of the proposed method is first demonstrated using a 3D unit pore as shown in Figure 4(a). Figure 5(a) shows that when a regular spherical structuring element is used, the pore body appears to be drained at pore diameter $d = 18$; yet at $d = 17$, the saturation jumps higher and the pore body is filled again. This is of course not a correct solution as the diameter of the top pore throat is measured at 16 voxels. Therefore, the pore body should only be drained when the diameter of the structuring element is less than or equal to 16 voxels. A similar result is observed for the wetting curve. Using the modified spherical structuring element as in (12) appears to fix this problem. The pore body is shown to be emptied at $d = 16$ for drainage and be filled at $d = 33$ for wetting, see Figure 5(b). However, monotonicity is still not being satisfied at $d = 25–27$, and at some other parts on the drainage curve. The use of modified structuring element can alleviate the problem of non-monotonicity but it fails to completely correct it (Hilpert & Miller 2001). Based on these results, the use of the modified sphere is recommended in this algorithm. The visualization of the drainage and wetting of the 3D convergent–divergent unit pore is shown in Figure 4(b) and (c), respectively. It should be mentioned that the surfaces being visualized in Figure 4 have been smoothed for ease of viewing; the original data consist of binary voxels that can be represented as cubes shown in Figure 3.

A simple pore network is also used to test and demonstrate the three types of drainage mechanisms implemented in the proposed algorithm. Type I drainage does not consider
WP entrapment explicitly and the algorithm assumes that the porous medium is totally wet and that a thin film of WP always coats the solid phase. Isolated pockets of WP at the corners and recesses of the pore space are in fact connected to the WP reservoir and respond uniformly to the changing of capillary pressure. They continue to drain and decrease in volume with rising pressure as demonstrated in Figure 6(a). For Type II drainage, all disconnected WP is drained. As a result, no isolated pockets of WP can be found at the corners of the drained pore space, see Figure 6(b). Figure 6(c) shows the Type III drainage where the WP is trapped once it is disconnected from the WP reservoir. The disconnected pockets of WP maintain their volume despite increasing pressure. As interpreted in the context of water retention curve, the Type III and Type II drainage results represent the upper and lower bound solutions. Type I results lie within these bounds.

Two types of wetting algorithms are demonstrated in Figure 7. Type I wetting does not consider NWP entrapment. The invasion of WP proceeds with decreasing pressure (larger diameter of structuring element) as observed in Figure 7(a). The interface advances if the diameter of its curvature exceeds the width of the widest opening ahead. Since the NWP cannot be trapped, an isolated pore space already surrounded by WP (i.e. disconnected from the NWP reservoir) can be filled if the aforementioned condition is satisfied, as noted from \( d = 60 \) to \( d = 90 \) in Figure 7(a). One potential problem with this wetting strategy is the inconsistency with assumptions made in Type I drainage—in particular, the existence of WP films that are connected to the WP reservoir at all times. Also some other mechanism, e.g. bubbling, has to be assumed for the escape of the NWP that is trapped in isolated pore space such as the one shown at \( d = 60 \) in Figure 7(a). Type II wetting allows for NWP entrapment, see Figure 7(b); however, it also runs into the same inconsistency that Type I wetting does. Moreover, the occurrence of trapped NWP appears to strongly depend on the resolution. Again, Type I and Type II wetting provide the upper and lower bound solutions, respectively.

**Fully penetrable spheres system**

Figure 8 shows the simulated drainage and wetting curves for an FPS system. The FPS porous medium used has a porosity, \( \phi \), of 0.35 and the particle-size characteristics of \( \mu_y = 3.5 \) and \( \sigma_y = 0.5 \). It is realized with a sample size of 1.53 mm\(^3\) and is discretized into a cube with 2503 voxels. Type I, Type II, and Type III drainage simulations were performed on the digital porous medium assuming water is the WP fluid and air is the NWP. Type I and Type II wetting simulations were also carried out. The capillary pressure, expressed in terms of
the pressure head of water, was calculated using the Laplace equation:

\[ h = \frac{2c}{d}, \text{ where } c = \frac{2n \cos \gamma}{\nu g} \]  

(22)

For room temperature and an assumed contact angle of zero, \( c \) is equal to 0.149 cm².

Results of the three types of drainage are mostly the same for saturations ranging from 0.2 to 1 (Figure 8). It is only at low saturations that differences among the drainage types can be discerned. Since no WP entrapment is considered in Type I and Type II drainage, both types result in complete drainage. Type II drainage predicts a zero saturation at a lower
pressure head because it assumes that once the WP is disconnected from the WP reservoir, it is completely drained. Type III drainage allows for WP entrapment, and as a result, the simulated curve shows an irreducible water saturation of slightly less than 0.1. As expected, the Type I drainage curve is bounded by Type II and Type III curves.

The wetting simulations assume the porous medium completely devoid of WP initially; therefore, both Type I and Type II wetting curves begin with zero saturation at high capillary pressure. Both wetting curves demonstrate hysteresis but while the Type I curve eventually joins the drainage curve at near saturation, the Type II curve achieves maximum saturation at slightly above 0.5. The Type II algorithm includes the NWP entrapment; however, it would appear that the algorithm has exaggerated the amount of NWP being trapped. The assumption that the trapped NWP maintains its volume with reducing pressure head is not entirely valid. It produces a less than desirable lower bound for the wetting curve.

Resolution effects

The resolution effect is studied by comparing the retention curves for Type I drainage using different degrees of discretization. The FPS porous medium used has the following parameters: \( \mu_p = 5.589 \), \( \sigma_p = 0.4512 \) and \( \phi = 0.3 \). The sample size of the medium is 1 mm\(^3\). The first apparent effect of resolution is on the number of resulting data points on the retention curve. The higher the resolution, the higher the density of data points that can be obtained from the simulations (see Figure 9). This is especially crucial around the inflection point of the retention curve, particularly for the drainage curve, where the change in saturation is large for a slight variation in capillary pressure. With a coarse resolution, important details in that portion of the retention curve will be lost. A tradeoff, however, is that higher resolution requires a significantly higher computation time.

For the drainage curve, the effect of resolution is more significant in the dry region of the retention curve as shown in Figure 9(a). Higher resolution results in a longer tailing at low saturation. Since Type I drainage is used, such a long tail results from the decreasing volume of WP at the corners and recesses of the pore space. Consequently, the higher the resolution, the better these volumes are resolved. However, the algorithm only accounts for capillary forces; in reality, drainage at low saturation also depends on other mechanisms such as adsorption, evaporation, etc. Further, at low saturation, the WP tends to be in pendular form for which the general form of the Young–Laplace equation applies. Significant error can result from assuming a spherical interface (Hilpert & Miller, 2001). The existence of WP film is not accounted for in this approach. The interpretation of the simulation results at the dry region should, therefore, be made with caution. Some scatter is also observed in the vicinity of the saturated portion of the drainage curve. Such scatter can be caused by the fact that each discretization level used a different realization of the porous medium. Overall the resolution effect on the drainage curve appears to be small.

For the wetting curve, the effect of resolution can be clearly seen also at the dry portion of the retention curve (Figure 9(b)). Increasing resolution is accompanied by longer tailing at low saturation. The lack of resolution fails to pick up smaller openings that govern the invasion of the WP. As the resolution increases, the smaller pores are better resolved and the corresponding pressure head for wetting increases. Resolution, for the range of values investigated, seems to have negligible effects over other parts of the wetting curve.
Sample-size effects

The sample-size effect is also investigated using the same FPS medium configuration realized with various sample sizes of fixed resolution. For the drainage curve, a larger sample size results in a sharper and more well-defined air-entry point and also a flatter shoulder that corresponds to a sharper drop in saturation at the inflection point, see Figure 10(a). This result is consistent with previous work by Hilpert & Miller (2001) and Dalla et al. (2003) on pore-morphology-based simulations and by Larson & Morrow (1981) on pore-network simulations (see also Mishra & Sharma 1988). In the saturated region, the decrease in saturation is mainly due to the drainage occurring at the top surface of the porous medium where it is connected to the NWP reservoir. Increasing the sample size will increase the area of the top surface, but at the same time, the pore volume increases at a much faster rate. Since the drainage is confined to only the top surface, the decrease in saturation for smaller samples is larger than that for larger samples. At the dry region, where the breakthrough of the NWP has already taken place (in the case, for $h > 70$ cm), the decrease in saturation is mainly due to the drainage of “isolated” pockets of WP residing at the
corners and recesses of the pore space. The ratio of the volume occupied by the isolated WP (to the total pore volume) is higher in smaller samples than in larger samples. Combining these two observations, one can fully explain the difference in the shape of the retention curve due to sample size in Figure 10(a).

The sample size has similar effects on the wetting curves. Increase in saturation, at the dry range, is slightly higher for smaller samples, see Figure 10(b). The same explanation for drainage at near saturation applies here. The observed difference is small because the change of volume is much smaller due to WP invasion of a dry porous medium than the drainage of a saturated one. At the saturated region, a few “hold-out” (larger WP-filled) pores in the smaller samples account for a relatively higher percentage of pore volume than in the larger samples. As a result, the increase of saturation at the near saturation region is more gradual for smaller samples.

Scanning curves

To simulate scanning curves, the primary drainage and wetting curves (both Type I) were first generated using the FPS porous medium with parameters: \( \mu_y = 3.589 \), \( \sigma_y = 0.4512 \), and \( \phi = 0.3 \). The sample size of the medium was 1 mm\(^3\) and was discretized into a cube of 2003 voxels. For each point simulated on the retention curves, the NWP configuration was saved and later used as the initial condition for the simulation of the scanning curves. Each drainage scanning curve was obtained using one of the points on the primary wetting curve as the starting position. Similarly, each wetting scanning curve was started from one of the simulated points on the primary drainage curve (Figure 11). The shape of the drainage scanning curves closely resemble that of the primary drainage curve while the wetting scanning curves resemble the primary wetting curve. The two primary curves serve as the bounds that contain all the scanning curves.

INTERFACIAL AREA RESULTS

Simple objects

Mullikin & Verbeek (1993) and Windreich et al. (2003) both have evaluated the performance of the voxel-based surface area estimator using synthetic spheres. The use of spheres can reveal possible bias of the estimator. Since Dalla et al. (2002) have also used spheres to test their marching-cube algorithm, results from the voxel-based surface estimator and the marching-cube algorithm can be compared directly.

Figure 12(a) shows the relative errors in estimating the surface area of spheres using the voxel-based method. Each point on the graph was obtained by averaging the estimated surface area of 50 spheres for which the centers were randomly placed within a unit voxel. The error decreases dramatically from around 1.2% to less than 0.1% within the radii of 10 pixels. For radii larger than 20 pixels, the error is less than 0.04%. There is a slight overestimation at larger radii; however, for all practical purposes, this error is insignificant. Comparing these results with the ones obtained by marching-cube algorithm (Dalla et al. 2002), see Figure 12(b), it is apparent that the voxel-based method is a superior one. The surface area estimates produced by the marching-cube algorithm tend to have a much larger error at smaller radii. For larger radii, the bias is large and the error never drops below 8.4%.

Another test for the surface area estimator is that of a meniscus in a capillary tube. A contact angle of zero is assumed and the meniscus is therefore a perfect hemisphere with a diameter equal to that of the capillary tube. The voxel-based method is used to estimate the surface areas of the meniscus and the total NWP area for various sizes of the capillary tube. The total NWP area includes that of the
meniscus and a portion of the capillary tube. Figure 13 shows some interesting results on the estimated meniscus area by the voxel-based method. For smaller diameters (less than 20 voxels), the method underestimated the meniscus area. At around 20 voxels, the relative error becomes zero; however, the error increases as diameter increases. For larger diameters, the overestimation seems to stabilize at around 10%. The error of the estimated NWP area, on the other hand, stays constant at around 1.4% regardless of the size of the capillary tube. The discrepancy in the meniscus area is due to the difficulty in determining the exact termination point of the meniscus at the solid phase, the estimation of the meniscus area is subject to systematic bias. Overall, the voxel-based method is expected to yield a consistently higher precision than the marching-cube algorithm.

Fully penetrable spheres systems

The investigations on simple objects have shown that the voxel-based surface estimator provides very accurate estimates for the total NWP and SP surface areas. Due to the problem with the algorithm in resolving the termination point of the meniscus at the solid phase, the estimation of the meniscus area is subject to systematic bias. Overall, the voxel-based method is expected to yield a consistently higher precision than the marching-cube algorithm.

The accuracy of the voxel-based surface estimator is further analyzed using FPS systems. Realizations of a FPS porous medium of sample size 3 mm$^3$ and parameters $\mu_y = 3.5$, $\sigma_y = 0.5$, and $\phi = 0.35$ were used. Various levels of discretization (503 to 6503 voxels) were employed to investigate the effect of resolution on the accuracy of the surface estimator. Each data point on Figure 14a was obtained by averaging 30 realizations of the specified medium. The dotted line indicates the theoretical value of the specific surface area, which is obtained by

$$a_s = -\frac{3\phi m_2}{m_3} \ln \phi$$

where

$$m_n = \exp \left( n\mu + \frac{n^2 \sigma^2}{2} \right)$$

Figure 14(a) shows that the voxel-based method consistently underestimates the specific surface area of the medium;
however, as resolution increases, the estimation also improves. The error is due to both the inherent limitation of the method at low resolution (as shown in the previous section) and also the loss of spheres less than 1 voxel during the simulation of the FPS medium. Figure 14(b) shows that the estimated porosity values from the realizations are higher than the specified value used for generation.

**Resolution effects**

To investigate the resolution effects on the interfacial area estimates, the drainage and wetting simulation results of Figure 9 were used and the meniscus area, $a_{wm}$, and the total NWP area, $a_n$, were estimated from the NWP results for each point on the retention curves. Note that $a_n$ is equivalent to the total interfacial area between WP and NWP for Type I drainage because a fully wetting porous medium is assumed. Figure 15 plots the $a_{wm}$ and $a_n$ as a function of saturation. For both drainage and wetting, the values of $a_n$ tend to be largely unaffected by the level of resolution except for the lowest resolution at 503 voxels and at the dry portion of the curve. At low saturation, higher resolution is required to capture the angular pore corners. The effect of resolution observed here at the dry region is clearly demonstrated in Figure 14. At zero saturation, $a_n$ should be the same as the specific surface area of the porous medium, in this case, 18 mm$^{-1}$. As resolution increases, the value of $a_n$ at zero saturation approaches the theoretical value of the specific surface area.

The meniscus area (see (23)), on the other hand, is strongly affected by resolution stemming from the failure of the surface estimator to resolve the WP film at the vicinity of the SP–WP–NWP contact point. The results suggest that the $a_{wm}$ estimates are not reliable and should be used only for investigating trends in data.

**Sample-size effects**

The estimated values of $a_{wm}$ and $a_n$ shown in Figure 16 are based on drainage and wetting simulation results from Figure 10. Figure 16 shows that the sample size has little effect on the interfacial area (regardless of $a_{wm}$ or $a_n$) and saturation relationship, except for the smallest sample of 0.5 mm$^3$. Since the saturation and the specific surface area are both normalized by the volume of the medium while the capillary pressure head is not, sensitivity to sample size therefore only manifests in the capillary pressure relationship but not in the saturation.

**COMPARISON WITH THE FPS WATER RETENTION CURVE MODEL**

In this section, results obtained from the pore-morphology-based drainage simulation are compared with the prediction of the FPS soil water retention model developed by Chan & Govindaraju (2004). The premise of the FPS model is that one can infer the pore-size distribution from particle-size data of a soil. This is based on the assumption that a
coarse-textured soil can be idealized as a system of fully penetrable spheres—randomly placed in space—whose size distribution is lognormal. Figure 17 shows the Type I drainage simulation results using three FPS porous media with particle-size parameters: $\mu_y = 2, 3, 4$; $\sigma_y = 0.5$; $\phi = 0.35$. From Chan & Govindaraju (2004), the FPS model describes the retention curve with the following equation:

$$\Theta(h) = 1 - \exp \left\{ \ln\phi \left( \frac{c}{2h} \right)^3 + 3 \left( \frac{c}{2h} \right)^2 m_1 + 3 \left( \frac{c}{2h} \right) m_2 + m_3 \right\}$$

(25)
where \( a \) is a scaling factor that accounts for the bias resulting from how the pore size is defined and measured in the model.

The simulation results captured the trend of the FPS model (see Figure 17). The FPS model predicted a steeper curve but the simulation produced a retention curve with a much milder slope. The two curves cross at saturation of slightly higher than 0.2. The possible reasons for the mismatch of the model and the simulation results are postulated below. The inferred pore-size distribution in the FPS model is measured as the distribution of the distance from a randomly selected point in the void space to the nearest solid surface. This distance measurement is a one-dimensional quantity; thus the pore-size distribution is, in essence, a number distribution. To translate this distribution into a volume distribution of the pore size, the scaling factor \( a \) was introduced assuming that the distance measure is related to the pore size (radius) in a linear fashion. This linear relationship between the number distribution and the volume distribution is a weak approximation of the complex geometry of the pore structure and the difficulty in defining what constitutes a pore or a pore-throat. Even if such a relationship were known, there remains a problem of lack of connectivity information in the FPS model. The Laplace equation translates the corresponding capillary pressure. Directly applying it to the pore-size distribution implicitly assumes that each pore drains individually; thus the pores are not interconnected. As one can observe from previous simulation results, connectivity plays an important role in the drainage of a porous medium. In fact, the consideration of pore connectivity is central to the algorithm of the pore-morphology-based simulation technique. The failure of incorporating connectivity into the development of the theoretic model results in significant errors in predicting the retention curve. Further research is required to address these problems.

**ROLE OF INTERFACIAL AREA IN THE CONSTITUTIVE RELATIONSHIP**

Figure 18 shows a hysteretic relationship between meniscus area and saturation and also between meniscus area and pressure. The maximum meniscus area (5.4 mm\(^{-1}\)) was attained on one of the wetting scanning curves at a saturation of about 0.3 (which corresponds to a capillary pressure head of \( \approx 60 \) cm). In general the meniscus areas on the primary wetting curve are higher than those on the primary drainage curve, except in the dry region. This can be clearly seen in Figure 18(b) where capillary pressure head is plotted on a log scale. Most of the values of the meniscus area seem to be bounded by the primary drainage and wetting curves. This is contrary to Reeves & Celia’s (1996, Figures 8 and 9) simulation results using pore-scale network model, where their meniscus area–saturation scanning curve rises much higher than the ones for primary drainage and wetting. One has to consider that the pore geometry is represented differently in the pore-morphology-based approach and the network model.

The relationship between interfacial area, capillary pressure, and saturation (Figure 19) shows a strong functional dependence between covariates (Hassanizadeh & Gray 1990). The hysteretic behavior of the retention curve on the \( h-\Theta \) plane can be explained by \( a_{w} \). In fact, hysteresis is not limited to the retention curve (\( h-\Theta \) relationship) but it also occurs in the \( a_{w}-h \) and the \( a_{w}-\Theta \) relationships as shown in Figure 18. Data from the drainage and wetting scanning curves combined to form a single, unique surface. While this supports the experimental evidence presented by Cheng et al. (2004) on micro-models, it differs slightly from the pore-network model simulation results by Reeves & Celia (1996). In Reeves & Celia’s (1996) study, they obtained different surfaces from the drainage scanning curves and from the wetting scanning curves. Note that Type I drainage and wetting were used in the pore-morphology-based approach, where there is no explicit accounting for NWP or WP entrapment. But in Reeves and Celia’s network model,
the NWP entrapment is considered during wetting while the WP entrapment is not due to the assumption of a strongly wet medium, and could have resulted in the discrepancy between the surfaces generated by the drainage and wetting scanning curves. Reeves & Celia (1996) have also alluded to similar explanations in their paper.

Despite the ability of the pore-morphology-based approach to demonstrate the important role of interfacial area in the constitutive relationships, the simulation results and the interfacial areas estimated should be interpreted with caution. In an effort to simplify the fluid displacement mechanism, only capillary forces due to Laplace equation are considered. In fact, Cheng et al. (2004) have shown that the distribution of interfacial curvature is not uniform and not all interfaces are concave. A set of interfaces is dominated not by capillary pressure, but by disjoining pressure associated with the proximity to the solid surface. Particularly in low saturation conditions, adsorption begins to play a more dominate role in governing the constitutive relationships of drainage and wetting. Also, the accuracy of the meniscus interfacial area estimates remains questionable. Resolution effects should be considered in interpreting the results.

**CONCLUDING REMARKS**

The pore-morphology-based method, originally proposed by Hilpert & Miller (2001) for drainage simulations, was significantly extended to incorporate the ability to simulate wetting processes. As a result, the extended algorithm can now simulate intermediate scanning curves as well as hysteresis loops.
A voxel-based approach was also introduced to estimate surface areas of various interfaces in 3D media. The primary goals were to employ the proposed simulation technique to examine the proposed water retention models, and to investigate the role of interfacial area in the constitutive relationship of capillary pressure and saturation. The following conclusions are drawn from the results obtained in this work:

- The ink-bottle effect can be demonstrated by the proposed algorithm for simple objects as well as for the FPS systems. The pore-morphology-based technique, compared to other pore-scale modeling approaches, excels in its ability to fully consider the geometry of the pore structure.
- Type I drainage does not consider WP entrapment explicitly. Type II drainage assumes that all disconnected WP is drained, and Type III drainage considers WP entrapment. Drainage simulation results suggested that Type I drainage curve is bounded by Type II and Type III curves as the lower and upper bound solutions, respectively.
- Type II wetting includes NWP entrapment. However, this wetting algorithm appeared to have exaggerated the amount of NWP being trapped during the wetting of a FPS porous medium.
- The overall effects of resolution seem to be small. Other than the apparent effect of increasing data density with increasing resolution, the level of resolution has a small influence at both the wet and dry regions of the wetting curve.
- For drainage, increasing sample size results in a sharper and more well-defined air-entry point, along with a flatter shoulder that corresponds to a sharper drop in saturation at the vicinity of the inflection point. Sample size has a similar effect on the wetting curve.
- The voxel-based surface area estimator was shown to produce more accurate interfacial area estimates than the marching-cube algorithm.
- The lack of resolution near the WP–NWP–SP contact point strongly affects the accuracy in estimating the meniscus area and is further challenging at low saturation.
- The FPS retention model failed to predict the drainage simulation results. Interestingly, the effect of hysteresis for \( a_s(\theta) \) appeared to be much smaller than that for \( a_s(h) \). The cause is unclear, however, a similar phenomenon is often observed in the hydraulic conductivity function.

Future research is necessary to improve on the speed of the drainage–wetting simulator. Also, the current methodology limits the accuracy and application of the simulator at high capillary pressures. The impact of pendular WP and WP films should be considered. Further verification of the wetting algorithm using experimental data is desirable.

REFERENCES


First received 14 May 2009; accepted in revised form 27 November 2009. Available online February 2011.
APPENDIX

List of symbols

\( \alpha_s \) Specific surface area (L\(^{-1}\))

\( \alpha_n \) NWP surface area (L\(^{-1}\))

\( \alpha_{m} \) Meniscus surface area (L\(^{-1}\))

\( c \) Constant = 0.149 cm\(^2\) or center of a digital 3D sphere in (4)

\( C \) Connectivity analysis using a 3D six-connected neighborhood or set complement if appeared as a superscript

\( d \) Size of structuring element or equivalent pore diameter (L)

\( d_{\text{max}} \) Maximum particle diameter for RC model (L)

\( D \) Diameter (L)

\( \Theta \) Effective water saturation

\( \Theta_{n} \) NWP effective saturation

\( \Theta_{w} \) WP effective saturation

\( \gamma \) Scaling factor for RC model

\( \delta \) Empty or null

\( e \) Number density of spheres per unit volume (L\(^3\) L\(^{-3}\))

\( g \) Gravitational acceleration (LT\(^{-2}\))

\( h \) Capillary pressure, expressed in terms of the pressure head of water (L)

\( h_{\text{p}} \) Pressure head of water (L)

\( i \) Dimension or class member of surface voxel

\( j \) Proper subset

\( k \) Belongs to

\( k \) Minkowski subtraction

\( k \) Set union

\( m_{n} \) \( n \)th moment for a log-transformed size distribution in (24)

\( m_{i} \) Number of surface voxels belonging to the \( i \)th class

\( \mathbb{N}_{i} \) Morphological opening

\( \mathbb{O} \) Morphological erosion

\( \mathbb{P} \) Pore space

\( \mathbb{P}_c \) WP-filled pore space that is connected to the WP reservoir

\( \mathbb{P}_e \) Eroded pore space

\( \mathbb{P}_{ce} \) Eroded pore space that is connected to the NWP reservoir

\( \mathbb{P}_{dcw} \) Disconnected pockets of WP

\( \mathbb{P}_{n,ex} \) Existing (initial condition) of the NWP-filled pore space

\( \mathbb{P}_{n} \) NWP occupied pore space

\( \mathbb{P}_o \) Opened pore space

\( \mathbb{P}_w \) WP occupied pore space

\( \mathbb{r} \) Distance vector

\( \mathbb{S} \) Structuring element

\( \mathbb{S}' \) Modified structuring element

\( \mathbb{S}_\mathbb{r} \) Total surface area estimator

\( \mathbb{W}_i \) Weight of the \( i \)th class of surface voxel

\( \mathbb{X} \) Set

\( \mathbb{Y}_{n} \) NWP effective saturation

\( \mathbb{Y}_{w} \) WP effective saturation

\( \mathbb{Z}^3 \) Discrete space for a cubic lattice

\( \emptyset \) Empty or null

\( \pi \) Constant, ratio of a circle’s circumference to its diameter

\( \rho \) Density of water (ML\(^{-3}\))

\( \mu_{y} \) Mean of the log-transformed particle size distribution

\( \sigma \) Standard deviation of the log-transformed particle size distribution

\( \phi \) Porosity of the porous medium

\( \psi \) Contact angle (assumed zero)

\( \Theta_{n} \) NWP effective saturation

\( \Theta_{w} \) WP effective saturation

\( \gamma \) Scaling factor for RC model

\( \delta \) Empty or null

\( e \) Number density of spheres per unit volume (L\(^3\) L\(^{-3}\))

\( s \) Surface tension (MT\(^{-2}\))