Comparison of Average and Point Capillary Pressure–Saturation Functions Determined by Steady-State Centrifugation

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The capillary pressure–saturation function can be determined from centrifuge drainage experiments. In soil physics, the data resulting from such experiments are usually analyzed by the "averaging method." In this approach, average relative saturation, $\langle S\rangle$, is expressed as a function of average capillary pressure, $\langle\psi\rangle$, i.e., $\langle S\rangle(\langle\psi\rangle)$. In contrast, the capillary pressure–saturation function at a physical point, i.e., $S(\psi)$, has been extracted from similar experiments in petrophysics using the "integral method." The purpose of this study was to introduce the integral method applied to centrifuge experiments to a soil physics audience and to compare $S(\psi)$ and $\langle S\rangle(\langle\psi\rangle)$ functions, as parameterized by the Brooks–Corey and van Genuchten equations, for 18 samples drawn from a range of porous media (i.e., Berea sandstone, glass beads, and Hanford sediments). Steady-state centrifuge experiments were performed on preconsolidated samples with a URC-628 Ultra-Rock Core centrifuge. The angular velocity and outflow data sets were then analyzed using both the averaging and integral methods. The results show that the averaging method smoothes out the drainage process, yielding less steep capillary pressure–saturation functions relative to the corresponding point-based curves. Maximum deviations in saturation between the two methods ranged from 0.08 to 0.28 and generally occurred at low suctions. These discrepancies can lead to inaccurate predictions of other hydraulic properties such as the relative permeability function. Therefore, we strongly recommend use of the integral method instead of the averaging method when determining the capillary pressure–saturation function by steady-state centrifugation. This method can be successfully implemented using either the van Genuchten or Brooks–Corey functions, although the latter provides a more physically precise description of air entry at a physical point.

The capillary pressure–saturation function is an important hydraulic property of variably saturated rocks and soils. This function is needed for simulating multiphase fluid flow and chemical transport in porous media in applications such as agricultural crop production, enhanced oil recovery, subsurface C sequestration, and remediation of contaminated soils. In soil physics, the capillary pressure–saturation function is traditionally determined in the laboratory using a hanging water column (Dane and Hopmans, 2002a) or pressure plates (Dane and Hopmans, 2002b). In these methods, a series of capillary pressures, ψ, are imposed at a particular point and the corresponding volumetric water contents for the entire porous medium, $\langle\theta\rangle$, are determined gravimetrically or manometrically. If the densities of the nonwetting and wetting fluids are different, ψ will vary with height within the porous medium (Dane et al., 1992; Liu and Dane, 1995a). As a result, the volumetric water content at the point where ψ is controlled, θ, can deviate significantly from the measured $\langle\theta\rangle$. Thus, use of the capillary pressure–average saturation function, $\langle\theta\rangle(\psi)$, instead of the point capillary pressure–saturation function, $\theta(\psi)$, in flow and transport models can produce erroneous predictions of important hydraulic properties such as the relative permeability function (Peters and Durner, 2006).

Because point measurements of θ are rarely available in hanging water column and pressure plate experiments, computational procedures have been developed to extract the $\theta(\psi)$ function from the measured $\langle\theta\rangle(\psi)$ function. Liu and Dane

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(1995a,b), Jalbert et al. (1999), and Dane and Hopmans (2002c) presented analytical expressions to account for variations in ψ with column height. Their approach, called TrueCell, corrects the parameters of the Brooks and Corey (1964) equation for the height of the experimental column given information about the pressure cell setup and fluid densities. Sakaki and Illangasekare (2007) successfully tested TrueCell against independent measurements of $\theta(\psi)$ made at a specific point in nine columns of sandy material. Jalbert and Dane (2001) proposed an alternative correction procedure that does not require the assumption of a particular equation for the $\theta(\psi)$ function. Because it is based on numerical derivatives, however, the method is highly sensitive to small fluctuations in the experimental data (Perfect et al, 2004). Despite these limitations, Tokunaga et al. (2002) were able to apply a special case of this procedure to obtain $\theta(\psi)$ functions for gravels. Schroth et al. (1996) introduced a more robust integral method to correct the parameters of the van Genuchten (1980) equation for column height. A numerical scheme was used to predict the $\langle\theta\rangle$, with the parameters of the point function estimated by least squares optimization against the measured $\langle\theta\rangle$ values. Peters and Durner (2006) generalized the numerical approach for arbitrary capillary pressure–saturation functions, including bimodal functions.

There is a long history in soil physics of using centrifuges to determine the capillary pressure–saturation function. Briggs and McLane (1907) were the first to use steady-state centrifugation to manipulate the water content of soil samples in drainage experiments. Later, Gardner (1937) measured ψ by determining the equilibrium water content of calibrated filter papers placed in contact with moist soil. The filter papers were calibrated by determining their water contents following equilibration at different angular velocities in a centrifuge. Russell and Richards (1938) were the first to construct the entire capillary pressure–saturation function by centrifuging soil samples; however, their data are actually $\langle\theta\rangle(\psi)$ functions. Khanzode et al. (2002) used essentially the same method to analyze their centrifuge data. The most recent approach has been to average the variation in ψ within the centrifuged sample, resulting in an average capillary pressure–average saturation function, $\langle\theta\rangle(\langle\psi\rangle)$ (Reatto et al., 2008). We refer to this method as the *averaging method*.

In contrast to the above studies, only two reports were found in the soil physics literature dealing with the integral method applied to centrifuge data. Odén (1975) appears to have been the first to extract a point $\theta(\psi)$ function from centrifuge experiments performed on soil samples. More recently, Peters and Durner (2006) derived the objective function for the integral fit of centrifuge data. They also performed a sensitivity analysis of the error of the averaging method.

In contrast to soil physics, the point $\theta(\psi)$ function has been routinely extracted from centrifuge drainage experiments in petrophysics. Numerous techniques for interpreting effluent outflow data obtained by steady-state centrifugation can be found in the petrophysics literature. Ruth and Chen (1995) and Forbes (1997) provided detailed reviews and comparative evaluations of the different computational procedures available. According to Christiansen (2001), these procedures can be divided into two main groups: differential and integral methods. Hassler and Brunner (1945) were the first to propose a method to calculate the point $\theta(\psi)$ function by differentiating the product of $\langle\theta\rangle$ and the point ψ. They adopted a graphical approach to determining the gradient. Numerical differentiation or fitting a differentiable equation to the observation data can also be used (Christiansen, 2001). The alternative integral method uses a parametric expression for the point $\theta(\psi)$ function to predict θ from known values of ψ at discrete points along the length of the sample. The resulting θ values are numerically integrated to give the $\langle\theta\rangle$ for a given angular velocity (ω). The calculated $\langle\theta\rangle$ values are then compared with the measured $\langle\theta\rangle$ values and, using an iterative least-square minimization technique, the parameters of the point equation are optimized. This one-dimensional integral method was originally described by Bentsen and Anli (1977). It is particularly versatile and attractive because it allows the incorporation of any parametric expression for the point $\theta(\psi)$ function (Christiansen, 2001). Although discussed in Peters and Durner (2006, Appendix A), this method does not appear to have been previously applied in a soil physics context. We refer to it as the *integral method*.

The objectives of this study were to: (i) introduce the integral method for determining the point $\theta(\psi)$ function with a centrifuge from the petrophysics literature to a soil physics audience, (ii) apply this method to extract point $\theta(\psi)$ functions for a range of porous media (Berea sandstone, glass beads, and Hanford sediments) using both the Brooks and Corey (1964) and van Genuchten (1980) equations, and (iii) compare the resulting point $\theta(\psi)$ functions with $\langle\theta\rangle(\langle\psi\rangle)$ functions for the same materials based on the averaging method of Reatto et al. (2008).

MATERIALS AND METHODS

Sample Preparation

The following porous media were selected for study: Berea sandstone (a consolidated siliciclastic rock from Ohio widely used as a standard material in petroleum engineering), packed glass beads (a commonly used "ideal" porous medium in soil physics), and unconsolidated, coarse-textured sediments collected from four different locations at the Environmental Restoration Disposal Facility (ERDF) on the U.S. Department of Energy's Hanford Reservation in the state of Washington. The Hanford sediments are of considerable environmental significance, and information about their point capillary pressure–saturation functions should be valuable for modeling the transport of transuranic waste in the Hanford vadose zone.

The Hanford samples consisted of both disturbed and undisturbed sediments. The disturbed sediments were the same as the fine- to medium-grained sand used in the flow and transport experiments reported by Pace et al. (2003) and Mayes et al. (2009) and referred to as HL (the same notation is used here). The other Hanford samples were all undisturbed cores excavated in August 2007 from an outcrop exposing three distinct sandy sedimentary layers (an upper coarse layer, UCL, a middle fine layer, MFL, and a lower coarse layer, LCL) at the ERDF. The undisturbed cores were obtained by first sculpting approximately cylindrical exposures of moist sediment, slightly larger than the desired sample dimensions. A cylindrical Delrin sample holder (3.31-cm diameter, 5.78-cm length) was then gently pushed over each sculpted exposure, resulting in a tight fit with minimal disturbance. The undisturbed cores were then temporarily sealed with impermeable caps. In the laboratory, these caps were replaced with permeable Delrin disks, perforated with 0.5-mm holes. Cheesecloth was placed between the sample and the bottom disk to prevent migration of fine-grained particles through the disk perforations during centrifugation.

The spherical soda lime glass beads (manufactured under the name Dragonite by Jaygo Inc., Union, NJ) were 45 to 70 μm in diameter, abbreviated as GB. The GB and HL samples were manually packed into the same Delrin sample holders that were used for collecting the undisturbed Hanford sediments. To minimize sample heterogeneity, both materials were moistened with de-aired water and added to the sample holders in ~5-mm layers. Each layer was tamped down with a glass rod and consolidated by lightly tapping several times on the sample holder. This process was repeated until each sample holder was full. The Berea sandstone samples were cylindrical rock cores (3.80-cm diameter, 4.78-cm length) supplied by Coretest Systems, Morgan Hill, CA, and did not require a sample holder. They were sleeved with Teflon tape to prevent the flow of water along the side of the core. Three replicate samples of each of these six materials (i.e., 18 cores) were selected for study.

All the samples were flushed with CO_2 for 0.5 h, saturated from the base with de-aired water for 12 h, and placed under a partial vacuum for 3 h while immersed in water. The relative saturations, $S \equiv \theta/\phi$, achieved by this method were ≥95%. The unconsolidated samples were precompacted by centrifugation at an angular velocity of 1047 rad s^{-1} (10,000 rpm) for 3 h to minimize any rearrangement of particles during the capillary pressure–saturation measurements. These samples were then resaturated following the same protocol as before. Next, the saturated hydraulic conductivity, K_{sat}, was determined with a constant-head permeameter following procedures similar to those presented in Reynolds and Elrick (2002). The combined resistance to flow of elements of the sample holder assembly (perforated plates, cheesecloth, tubes, etc.) was determined in separate experiments and its effect on the measured K_{sat} of the porous media was discounted. Dry bulk and particle densities were measured using gravimetry and pycnometry respectively, and then used to calculate the total porosity, ϕ (Flint and Flint, 2002). Particle size distributions were determined by combining hydrometer measurements with sieve analyses following the procedures outlined in Gee and Or (2002). The physical properties of the samples are summarized in Table 1.

Centrifugation

The saturated, precompacted samples were centrifuged with a URC-628 Ultra-Rock Core centrifuge (Coretest Systems, Morgan Hill, CA), described in detail by van den Berg et al. (2009). Each sample was subjected to several intervals of centrifugation at constant angular velocity, ω (Table 2). The ω values and their respective durations were selected based on drainage data from previous centrifuge experiments performed on extra samples of each material. For angular velocities <78.54 rad s^{-1} (750 rpm), a stabilizing arm was used to prevent excessive rotor wobble. For higher angular velocities, the rotor was stopped to remove this stabilizing arm and restarted within 5 min. The effect of this stoppage time on the fluid distributions was assumed to be minimal (Baldwin and Yamanashi, 1989).

The centrifuge rotor holds three samples fitted with effluent collection cups. During operation, the centrifuge automatically monitors the location of the air–water interface within each effluent collection cup. A dedicated data acquisition system converts the movement of this interface into a water volume–time series for each sample (van den Berg et al., 2009). These data were exported and used to compute the total volumes of water produced at equilibrium for each constant ω interval. The outflow data were then post-processed to correct for drainage from the perforated plates and cheesecloth during centrifugation. A second post-processing correction was applied to account for any discrepancy between the total outflow measured with the centrifuge and that obtained by weighing the samples before and after centrifugation.

Data Analysis

The average relative saturation, $\langle S \rangle$, associated with a given ω was calculated using

$$\langle S \rangle = \frac{PV - Q_w(\omega)}{PV} \quad [1]$$

where $Q_w(\omega)$ is the cumulative water outflow (mL) produced by that ω value and PV is the total pore volume of the sample (mL). The corresponding capillary pressure, ψ (Pa), at any point of interest along the radial through the center of the sample is given by (Christiansen, 2001)

$$\psi = \frac{1}{2}\Delta\rho\omega^2\left(r_o^2 - r^2\right) \quad [2]$$

Table 1. Physical properties of median grain diameter (d_{50}), porosity (ϕ), and saturated hydraulic conductivity (K_{sat}) for the Berea sandstone, glass beads (GB), and disturbed (HL) and undisturbed upper coarse layer (UCL), middle fine layer (MFL), and lower coarse layer (LCL) Hanford sediments investigated.

Sample–replicate no.	d_{50}	ϕ	K_{sat}
	μm	$m^3\ m^{-3}$	m s^{-1}
Berea-1	NA†	0.183‡	9.48×10^{-6}‡
Berea-2	NA	0.182‡	6.50×10^{-6}‡
Berea-3	NA	0.188‡	1.28×10^{-6}‡
GB-1	58§	0.367	6.26×10^{-5}
GB-2	58§	0.362	6.75×10^{-5}
GB-3	58§	0.360	6.83×10^{-5}
HL-1	98	0.413	5.34×10^{-5}
HL-2	98	0.415	3.43×10^{-5}
HL-3	98	0.411	4.18×10^{-5}
UCL-1	360	0.302	6.09×10^{-5}
UCL-2	400	0.346	1.46×10^{-4}
UCL-3	400	0.361	6.74×10^{-5}
MFL-1	310	0.322	1.64×10^{-4}
MFL-2	290	0.318	1.2×10^{-4}
MFL-3	290	0.321	1.81×10^{-4}
LCL-1	310	0.389	1.02×10^{-3}
LCL-2	410	0.396	4.32×10^{-4}
LCL-3	310	0.385	3.93×10^{-4}

† NA, not applicable for consolidated samples.
‡ Data supplied by Coretest Systems, Morgan Hill, CA.
§ Calculated as mean of upper and lower size bounds for fraction.

Table 2. Number and duration (t) of constant angular velocity (ω) periods used in the centrifuge experiments with Berea sandstone, glass beads (GB), and disturbed (HL) and undisturbed upper coarse layer (UCL), middle fine layer (MFL), and lower coarse layer (LCL) Hanford sediments.

Constant ω period	Berea		GB		HL		UCL		MFL		LCL	
	ω	*t*	ω	*t*	ω	*t*	ω	*t*	ω	*t*	ω	*t*
	s^{-1}	h	s^{-1}	h	s^{-1}	h	s^{-1}	h	s^{-1}	h	s^{-1}	h
1	51.4	5	36.7	12	49.7	12	41.9	6	49.7	6	41.9	6
2	78.5	5	41.9	12	57.6	12	49.7	6	57.6	6	49.7	6
3	104.7	5	49.7	12	62.8	12	57.6	6	78.5	6	57.6	6
4	130.9	4	57.6	12	73.3	12	68.1	6	104.7	6	68.1	6
5	157.1	7.5	62.8	12	83.8	12	83.8	6	209.4	6	83.8	6
6	209.4	7.5	73.3	12	94.2	12	104.7	6	418.9	6	104.7	6
7	314.2	7.5	83.8	12	104.7	12	209.4	6	628.3	3	209.4	3
8	418.8	7.5	94.2	12	130.9	12	418.9	6	942.5	3	733.0	3
9	523.6	10	104.7	12	157.1	12	628.3	6				
10	942.5	18	130.9	12	183.3	12	942.5	6				
11			157.1	12	209.4	12						
12			183.3	12	314.2	12						
13			209.4	12	523.6	12						
14			314.2	12	733.0	12						
15			523.6	12	942.5	12						
16			733.0	12								
17			942.5	12								

where $\Delta\rho$ is the density difference between the wetting and nonwetting fluids (kg m^{-3}), ω is the angular velocity (s^{-1}), r is the radial distance to any point on the axis of rotation of the cylindrical sample (m), and r_o is the radial distance to the effluent outlet (m). The average capillary pressure, $\langle\psi\rangle$ (Pa), for a sample subjected to a given ω was calculated from (Reatto et al., 2008)

$$\langle\psi\rangle=\frac{k}{6}\frac{\omega^2 L}{g}\left(L-3r_o\right) \quad [3]$$

where g is the acceleration due to gravity (9.81 m s^{-2}), k is a conversion factor equal to 9807 Pa m^{-1}, and L is the length of the sample (m).

The centrifuge data were parameterized using the "constrained" form of the van Genuchten (1980) equation:

$$S=\left(1-S_r\right)\left[1+\left(\alpha|\psi|\right)^n\right]^{-(1-1/n)}+S_r \quad [4]$$

where S_r is the residual saturation (dimensionless) and α (Pa^{-1}) and n are empirical parameters. For the averaging method, S and ψ in Eq. [4] were replaced with $\langle S\rangle$ and $\langle\psi\rangle$ from Eq. [1] and [3], respectively. Gauss–Newton nonlinear regression (SAS/STAT software, version 9.1.3, SAS Institute, Cary, NC) was then used to estimate the S_r, α, and n parameters in Eq. [4]. Point estimates of the same parameters were obtained using the integral method. Because detailed descriptions of the implementation of this method can be found in Schroth et al. (1996) for hanging water column or pressure cell experiments and in Bentsen and Anli (1977), Christiansen (2001), and Peters and Durner (2006) for centrifuge experiments, only an overview is provided here. Based on Eq. [2], the average relative saturation can be written in the following form:

$$\langle S\rangle(\omega)=\frac{1}{r_o-r_i}\int_{r_i}^{r_o} S\left[\psi(r,\omega)\right]\mathrm{d}r \quad [5]$$

where r_i is the radial distance to the air inlet (m). Because ψ is known for any location along the sample from Eq. [2] (we used $r = r_i$), best estimates of the van Genuchten parameters can be obtained by substituting Eq. [4] into Eq. [5] and minimizing the difference between the calculated and observed average saturations. Because point-based capillary pressure–saturation data are more likely to exhibit a distinct air-entry value, the Brooks and Corey (1964) equation may be more applicable than the van Genuchten (1980) equation when using the integral method. The Brooks and Corey equation (1964) can be written as

$$S=\left(1-S_r\right)\left(\frac{\psi_a}{\psi}\right)^{\lambda}+S_r \quad \left\{\psi>\psi_a\right\} \quad [6a]$$

$$S=1 \quad \left\{\psi\le\psi_a\right\} \quad [6b]$$

where ψ_a is the air-entry value (kg m^2 s^{-2}) and λ is the pore-size distribution index. Equation [6] was substituted into Eq. [5], and values of the S_r, ψ_a, and λ parameters were adjusted iteratively until the difference between the calculated and observed average saturations was reduced to a minimum. All of the integral method optimizations were performed using the Microsoft Excel spreadsheet program PcCentData from Christiansen (2001), which was modified to accommodate the van Genuchten (1980) and Brooks and Corey (1964) equations.

RESULTS AND DISCUSSION

Quasi-steady-state centrifuge experiments were performed on 18 samples as described above. Water drainage during centrifugation showed rapid adaptation to each stepwise increase in angular velocity followed by longer periods in which little water was produced as the hydraulic gradients approached equilibrium (Fig. 1). Outflow at high angular velocities (i.e., ω > 523.6 s^{-1}) was always very small compared with the amounts obtained in the preceding intervals. Estimates of saturation were based on

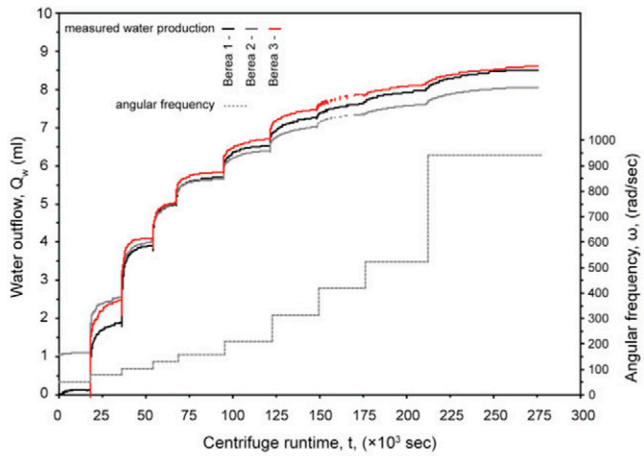

Fig. 1. Step changes in centrifuge angular velocity, ω (lower curve), and corresponding water outflow, Q_w (upper curves), through time for the three replicate samples of Berea sandstone.

the total volumes of water produced during each constant ω interval and assumed that hydraulic equilibrium was reached prior to increasing ω.

Application of the van Genuchten (1980) equation to the $\langle S \rangle$ vs. $\langle \psi \rangle$ data pairs obtained using the averaging method produced the suite of parameter estimates given in Table 3. Goodness of fit, as quantified by the RMSE, was generally very good, with a mean value of 1.52×10^{-2} and a maximum value of 2.43×10^{-2}. An example fit of the van Genuchten (1980) equation to the averaging method data is shown in Fig. 2.

In the integral method, the modeled $\langle S \rangle$ values were matched to the measured $\langle S \rangle$ values by iteratively adjusting the parameters of the van Genuchten (1980) equation using PcCentData (Christiansen, 2001). Figure 3 shows that a very good correspondence was achieved between the measured and modeled average relative saturations (denoted by the closed and open circles, respectively). The point-based function that gave the best fit between the measured and modeled $\langle S \rangle$ values is represented by the line in Fig. 3. It is important to stress that this function was obtained by optimizing Eq. [4] within Eq. [5] and not by direct fitting of Eq. [4] to the experimental data, hence the discrepancy between the line and the circles in Fig. 3. This is to be expected because the use of $\langle S \rangle$ values smoothes out the drainage curve. As a result, the van Genuchten (1980) function for a physical point (the line in Fig. 3) is much steeper than the corresponding function obtained by simply fitting the $\langle S \rangle$ values (the line in Fig. 2).

The mean and maximum RMSE values resulting from the point-based van Genuchten (1980) equation fits were 1.29×10^{-2} and 2.06×10^{-2}, respectively (Table 4). A paired *t*-test indicated that the mean RMSE value from the integral method was significantly lower than the mean value from the averaging method at the 95% confidence level. Thus, not only does the integral method provide a more accurate physical description of the drainage process than the averaging method, but it also provides a better fit to the experimental data.

Table 3. Summary of van Genuchten (1980) model fits and estimates of the residual saturation, S_r, and α and *n* parameters for the averaging method of Reatto et al. (2008) for the Berea sandstone, glass beads (GB), and disturbed (HL) and undisturbed upper coarse layer (UCL), middle fine layer (MFL), and lower coarse layer (LCL) Hanford sediments.

Sample	S_r	α	*n*	RMSE
		kPa^{-1}		
Berea-1	0.178	0.087	1.893	2.36×10^{-2}
Berea-2	0.160	0.131	1.671	8.11×10^{-3}
Berea-3	0.143	0.119	1.658	6.29×10^{-3}
GB-1	0.203	0.123	3.191	2.43×10^{-2}
GB-2	0.176	0.115	2.942	1.96×10^{-2}
GB-3	0.214	0.116	3.086	1.94×10^{-2}
HL-1	0.255	0.160	2.531	1.88×10^{-2}
HL-2	0.277	0.161	2.544	2.00×10^{-2}
HL-3	0.245	0.161	2.537	1.95×10^{-2}
UCL-1	0.097	0.276	2.177	1.52×10^{-2}
UCL-2	0.127	0.638	2.139	8.28×10^{-3}
UCL-3	0.119	0.553	2.140	6.16×10^{-3}
MFL-1	0.283	0.237	2.268	1.81×10^{-2}
MFL-2	0.273	0.290	2.131	1.35×10^{-2}
MFL-3	0.265	0.258	2.191	1.13×10^{-2}
LCL-1	0.097	1.237	1.856	1.32×10^{-2}
LCL-2	0.151	1.467	1.755	1.52×10^{-2}
LCL-3	0.127	1.376	1.782	1.22×10^{-2}

Best-fit estimates of the point-based van Genuchten (1980) equation parameters are summarized in Table 4. To facilitate comparison with the corresponding parameters from the averaging method, 1:1 plots were constructed for S_r, α, and *n* (Fig. 4–6). Estimates of the residual water content varied between 0.097 and 0.283 for the averaging method and between 0.093 and 0.273 for the integral method (Tables 3 and 4). There was a slight trend toward overestimation of S_r by the averaging method, but in general both sets of parameter estimates were very close to each other (Fig. 4). This is because the average relative saturation is quite similar to the point relative saturation at r_i for the high capillary pressures produced by high angular velocities (Fig. 3).

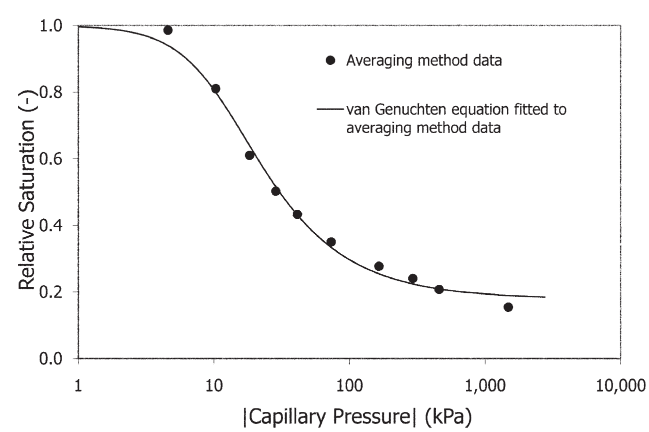

Fig. 2. Measured capillary pressure–saturation data and fitted van Genuchten (1980) function for the Berea-1 sandstone sample based on the averaging method of Reatto et al. (2008).

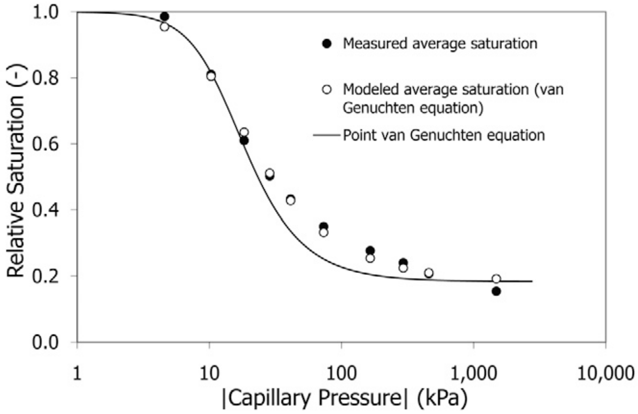

Fig. 3. Measured and modeled average saturations and resulting point van Genuchten (1980) capillary pressure–saturation function for the Berea-1 sandstone sample based on the integral method of Bentsen and Anli (1977).

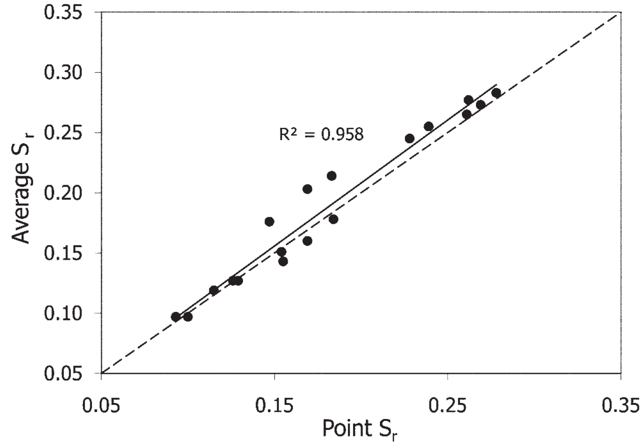

Fig. 4. Relationship between residual saturation (S_r) values in the van Genuchten (1980) capillary pressure–saturation equation estimated using the averaging and integral methods. The dashed line indicates a 1:1 correspondence.

Estimates of α varied between 0.087 and 1.467 kPa^{-1} for the averaging method and between 0.076 and 1.389 kPa^{-1} for the integral method (Tables 3 and 4). For low values of α (less than ~0.3 kPa^{-1}), both methods yielded similar estimates of this parameter (Fig. 5). The averaging method consistently overestimated the larger α values, however, compared with the integral method. The α parameter in Eq. [4] determines the location of the air-entry region on the capillary pressure–saturation curve. Thus, any overestimation of α will lead to a shift in the air-entry region toward lower suctions, with a corresponding overprediction of the diameter of the largest pores present. This effect was most pronounced for the coarse-textured UCL and LCL samples from Hanford.

Estimates of the dimensionless *n* parameter varied between 1.658 and 3.191 for the averaging method and between 1.913 and 9.523 for the integral method (Tables 3 and 4). Unlike the other two fitted parameters in Eq. [4], the *n* parameter showed a major curvilinear deviation from the 1:1 line for the two estimation methods (Fig. 6). The *n* parameter controls the steepness of the capillary pressure–saturation function as water drains at suctions >1/α; the larger the value of *n*, the steeper the curve. It is clear from Fig. 6 that the averaging method systematically underestimated this parameter relative to the point-based estimates. Any underestimation of *n* will lead to an overprediction of the breadth of the pore size distribution. The source of this bias is the averaging method's reliance on the $\langle S \rangle$ and $\langle \psi \rangle$ values, which in effect smoothes out measurements of the drainage process. The magnitude of the error introduced by this smoothing process will be greatest for coarse-textured materials in long sample columns (Dane and Hopmans, 2002c).

The Brooks and Corey (1964) function, Eq. [6], may be more applicable to point-based data than the van Genuchten

Table 4. Summary of van Genuchten (1980) model fits and estimates of the residual saturation, S_r, and α and *n* parameters for the integral method of Bentsen and Anli (1977) for the Berea sandstone, glass beads (GB), and disturbed (HL) and undisturbed upper coarse layer (UCL), middle fine layer (MFL), and lower coarse layer (LCL) Hanford sediments.

Sample	S_r	α	*n*	RMSE
		kPa^{-1}		
Berea-1	0.184	0.076	2.442	2.06×10^{-2}
Berea-2	0.169	0.120	1.920	9.30×10^{-3}
Berea-3	0.155	0.108	1.913	7.27×10^{-3}
GB-1	0.169	0.108	9.523	9.39×10^{-3}
GB-2	0.147	0.103	5.867	2.01×10^{-2}
GB-3	0.183	0.103	7.220	1.16×10^{-2}
HL-1	0.239	0.141	4.337	1.49×10^{-2}
HL-2	0.262	0.142	4.471	1.51×10^{-2}
HL-3	0.228	0.143	4.335	1.64×10^{-2}
UCL-1	0.093	0.239	3.195	9.57×10^{-3}
UCL-2	0.126	0.482	3.877	5.71×10^{-3}
UCL-3	0.115	0.457	3.269	7.95×10^{-3}
MFL-1	0.278	0.206	3.489	1.74×10^{-2}
MFL-2	0.269	0.249	3.107	1.36×10^{-2}
MFL-3	0.261	0.222	3.291	1.03×10^{-2}
LCL-1	0.100	1.062	2.354	1.38×10^{-2}
LCL-2	0.154	1.389	2.040	1.59×10^{-2}
LCL-3	0.129	1.272	2.109	1.29×10^{-2}

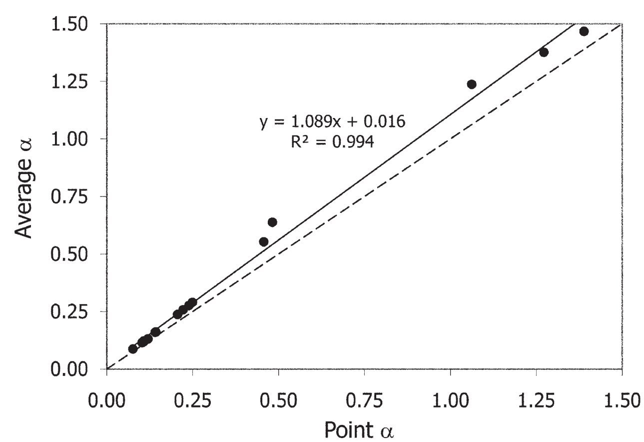

Fig. 5. Relationship between the α parameter in the van Genuchten (1980) capillary pressure–saturation equation estimated using the averaging and integral methods. The dashed line indicates a 1:1 correspondence.

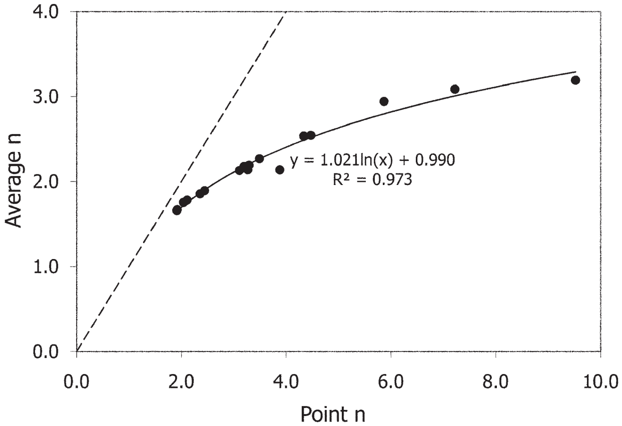

Fig. 6. Relationship between the *n* parameter in the van Genuchten (1980) capillary pressure–saturation equation estimated using the averaging and integral methods. The dashed line indicates a 1:1 correspondence.

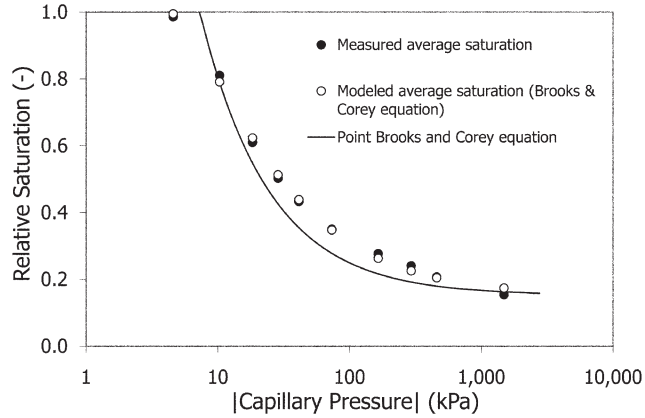

Fig. 7. Measured and modeled average saturations and resulting point Brooks and Corey (1964) capillary pressure–saturation function for the Berea-1 sandstone sample based on the integral method of Bentsen and Anli (1977).

(1980) function, Eq. [4]. This is because Eq. [6] is a segmented model that contains a distinct air-entry value, ψ_a, separating the saturated portion of the capillary pressure–saturation curve from the partially drained region. Theoretically, a sharp break is to be expected at a physical point, whereas an air-entry region, as represented by the α parameter in the van Genuchten (1980) equation, best describes the drainage process when it is averaged throughout a finite volume. To explore possible modeling variations between the Brooks and Corey (1964) and van Genuchten (1980) functions, the integral method was also implemented using Eq. [6] instead of Eq. [4] for comparison with the preceding results. The goodness-of-fit and parameter estimates are summarized in Table 5, with a typical result shown in Fig. 7. The mean and maximum RMSE values for Eq. [6] were 1.30×10^{-2} and 2.11×10^{-2}, respectively (Table 5). A paired *t*-test indicated no significant difference (at the 95% confidence level) between the mean RMSE values for Eq. [4] and [6] fitted to the integral method data for a physical point. We anticipated a better fit for Eq. [6] than for Eq. [4] for the reasons described above. The absence of any difference between the two models may be related to the limited number of data pairs in the low suction range.

Table 5. Summary of Brooks and Corey (1964) model fits and estimates of the residual saturation S_r, air-entry value ψ_a, and pore-size distribution index λ for the integral method of Bentsen and Anli (1977) for the Berea sandstone, glass beads (GB), and disturbed (HL) and undisturbed upper coarse layer (UCL), middle fine layer (MFL), and lower coarse layer (LCL) Hanford sediments.

Sample	S_r	ψ_a	λ	RMSE
		kPa		
Berea-1	0.152	7.298	0.827	1.26×10^{-2}
Berea-2	0.128	4.319	0.573	1.38×10^{-2}
Berea-3	0.137	9.700	0.694	1.36×10^{-2}
GB-1	0.168	7.695	4.798	1.10×10^{-2}
GB-2	0.145	7.354	2.881	2.11×10^{-2}
GB-3	0.181	7.663	3.515	1.28×10^{-2}
HL-1	0.235	5.021	2.066	1.33×10^{-2}
HL-2	0.258	5.057	2.134	1.32×10^{-2}
HL-3	0.225	4.995	2.086	1.49×10^{-2}
UCL-1	0.086	2.736	1.401	9.12×10^{-3}
UCL-2	0.125	1.650	2.384	5.24×10^{-3}
UCL-3	0.115	1.679	1.883	9.18×10^{-3}
MFL-1	0.277	3.467	1.781	1.78×10^{-2}
MFL-2	0.267	2.831	1.554	1.44×10^{-2}
MFL-3	0.259	3.183	1.655	1.10×10^{-2}
LCL-1	0.099	0.736	1.216	1.33×10^{-2}
LCL-2	0.154	0.569	0.954	1.53×10^{-2}
LCL-3	0.129	0.617	1.012	1.24×10^{-2}

Figure 8 compares the capillary pressure–saturation functions for the Berea-1 sample resulting from the three modeling approaches (averaging method with Eq. [4], integral method with Eq. [4], and integral method with Eq. [6]). The functions are clearly sensitive to the different modeling methods. Regardless of the equation used, the two point-based functions are similar at intermediate and high $|\psi|$ values, predicting more rapid drainage and lower saturations than the averaging method function. In contrast, at low $|\psi|$ values, the two van Genuchten (1980) functions (for the averaging and integral methods) are quite similar, while the point-based Brooks and Corey (1964) function exhibits a sharp break in slope at the air-entry value and higher relative saturation values.

Maximum deviations between the relative saturations predicted by the averaging and integral methods ranged from 0.078

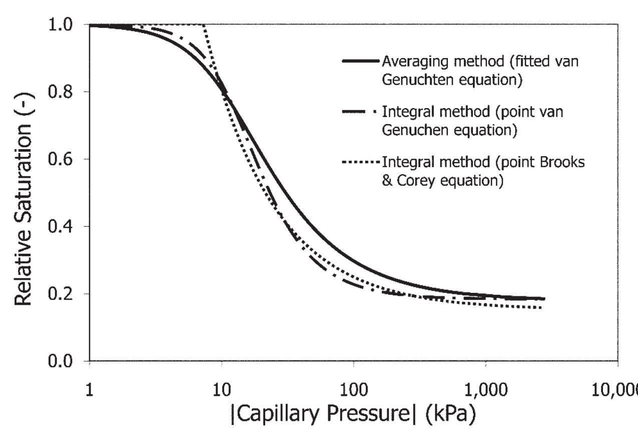

Fig. 8. Comparison of capillary pressure–saturation functions for the Berea-1 sample obtained using the averaging and integral methods.

Table 6. Maximum deviations in relative saturation (ΔS) between the averaging and integral methods for the Brooks–Corey (BC) or van Genuchten (VG) models for the Berea sandstone, glass beads (GB), and disturbed (HL) and undisturbed upper coarse layer (UCL), middle fine layer (MFL), and lower coarse layer (LCL) Hanford sediments.

Sample	Max. $\lvert\Delta S_{BC}\rvert$	Max. $\lvert\Delta S_{VG}\rvert$
Berea-1	0.078	0.098
Berea-2	0.083	0.063
Berea-3	0.083	0.066
GB-1	0.281	0.228
GB-2	0.258	0.224
GB-3	0.244	0.216
HL-1	0.177	0.139
HL-2	0.177	0.130
HL-3	0.171	0.140
UCL-1	0.129	0.137
UCL-2	0.164	0.145
UCL-3	0.158	0.133
MFL-1	0.156	0.127
MFL-2	0.130	0.114
MFL-3	0.127	0.110
LCL-1	0.133	0.107
LCL-2	0.115	0.096
LCL-3	0.115	0.093

to 0.281 (Table 6). The largest deviations were for the glass bead (GB) samples, which had the narrowest range of pore sizes. The smallest deviations were for the Berea sandstone samples, which had a relatively broad range of pore sizes. The point-based Brooks and Corey (1964) model produced higher maximum deviations than the point-based van Genuchten (1980) model in 14 out of the 18 samples investigated (Table 6). With the sole exception of the Berea cores, these maximum deviations occurred at $|\psi|$ values <10 kPa. For all of the samples, the maximum deviations observed for the Brooks and Corey (1964) equation occurred at suctions less than or equal to those at which the maximum deviations occurred for the van Genuchten (1980) equation. These trends can be attributed to the more precise representation of air entry at a physical point by the Brooks and Corey (1964) function.

Based on the above results, we recommend use of the integral method instead of the averaging method for determining the capillary pressure–saturation function using steady-state centrifugation. The use of the averaging method results in a smoothing out of the drainage process, which can lead to inaccurate predictions of other hydraulic properties such as the relative permeability function. The integral method clearly improves data evaluation and can be implemented with any parametric model. We used the "constrained" van Genuchten (1980) and Brooks and Corey (1964) models, which gave similar results, although the latter provides a more physically precise description of air entry at a physical point.

Reatto et al. (2008) reported an approximate one-to-one relationship between capillary pressure–saturation curves determined by steady-state centrifugation and those measured using the pressure plate method. Other researchers, however, have noted significant deviations between data sets obtained with these two methods (e.g., Omoregie, 1988; Khanzode et al., 2002). We suggest that the "good correspondence" observed by Reatto et al. (2008) was mainly due to the short column length used (5 cm) and the fine texture of most of their samples (average clay content of 460 g kg^{-1}). It may also be somewhat fortuitous due to the following confounding factors. First, their comparison was between centrifuged and noncentrifuged samples, and centrifugation is known to produce changes in the total porosity and pore size distribution relative to undisturbed material (Nimmo and Akstin, 1988). The effects of such changes on the capillary pressure–saturation function are well documented (Stange and Horn, 2005; Assouline, 2006). No mention was made of this important issue in the study of Reatto et al (2008). Second, their comparison was between centrifuge $\langle\theta\rangle(\langle\psi\rangle)$ curves and pressure plate $\langle\theta\rangle(\psi)$ curves. A more meaningful comparison would have been between the point $\theta(\psi)$ curves extracted from these two methods. Such a comparison is needed to document the effects of any centrifuge-induced compaction on soil water retention. In our opinion, the steady-state centrifuge method requires further investigation before it can be recommended for the routine measurement of capillary pressure–saturation curves on unconsolidated materials.

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