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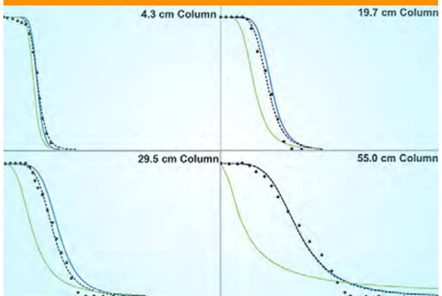
Original Research



Core Ideas

- The BC-vG Upscaler predicts the drainage of porous media of different heights.
- The default reference pressure elevation (RPE) is the middle of the porous medium.
- Predicted drainage functions deviate from observed functions as height increases.
- A top RPE improves accuracy of predicted drainage functions regardless of height.

Upscaling Capillary Pressure–Saturation Functions Using Different Reference Pressure Elevations

Chu-Lin Cheng, S. Clark Cropper,* Edmund Perfect, Larry McKay, and Misun Kang

Choice of reference pressure elevation (RPE) on average effective saturation–capillary pressure functions, $\langle \overline{S}_e \rangle(\psi)$, was investigated for monotonic drainage of homogeneous porous media. Nine columns of Flint sand with heights ranging from 4.3 to 55.0 cm were prepared. Measured $\langle \overline{S}_e \rangle(\psi)$ functions were determined gravimetrically using the hanging water column method. Predicted $\langle \overline{S}_e \rangle(\psi)$ functions were obtained by upscaling point function parameters determined by neutron radiographic imaging of a single drainage experiment. Bottom and midpoint RPEs resulted in the inaccurate parameterization of $\langle \overline{S}_e \rangle(\psi)$ functions for tall columns. A top RPE produced accurate upscaled functions for all column heights. To evaluate the overall performance of this RPE, observed effective saturations for the nine columns were linearly regressed against predicted values. The resulting best-fit model (slope = 0.98; intercept = 0.03; R^2 = 0.98) corresponded closely to a 1:1 line. The van Genuchten (vG) α and n parameters for the observed and predicted $\langle \overline{S}_e \rangle(\psi)$ functions decreased with increasing column height. A power model explained >95% of the variance in the predicted vG parameters and between 69 and 78% of the variance in the observed vG parameters. The lower R^2 values for the observed parameter models were attributed to experimental variation among the nine columns, whereas the predicted parameter models were upscaled from a single column. Despite these differences, the magnitudes and height dependencies of the observed and predicted average vG parameters were similar. For tall columns, the RPE should be established at the top for drainage experiments and at the bottom for wetting experiments.

Abbreviations: BC, Brooks and Corey; RPE, reference pressure elevation; vG, van Genuchten.

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The hydraulic properties of natural porous media, such as soil and rock, commonly display scale dependency. As a result, techniques are needed for up- and downscaling hydraulic properties to make predictions at one scale based on measurements made at another scale. Typical examples include the forward prediction of field-scale flow and transport processes based on laboratory measurements of hydraulic properties, and the inverse estimation of effective hydraulic parameters from the application of small-scale constitutive equations to field-scale data sets.

Vereecken et al. (2007) and Pachepsky and Hill (2017) reviewed various forward and inverse scaling techniques that are commonly used in vadose zone hydrology. It is clear from these reviews that there is a need for continued research on scaling methods. In particular, existing upscaling approaches, which rely on small-scale measurements to predict large-scale properties and processes, have not been extensively validated.

The capillary pressure–saturation function is a key hydraulic property used to characterize water retention in the vadose zone and to predict relative permeability. It is typically described by parametric models such as the Brooks and Corey (1964), BC, and van Genuchten (1980), vG, equations, which are used to provide model inputs when numerically simulating a variety of parameters related to energy and the environment (e.g., plant water use, pollutant transport, permafrost thawing, and carbon sequestration in confined brine aquifers).

Short columns often underrepresent the full range of physicochemical conditions in a particular soil horizon and thus may not constitute a representative elementary volume. However, because capillary pressure varies with height, the choice of a reference pressure elevation (RPE) (Liu and Dane, 1995; Dane and Hopmans, 2002) becomes significant when capillary–pressure saturation functions are measured on tall columns. Depending on the choice of RPE, both positive and negative values of capillary pressure can occur. This situation violates the definition of capillary pressure and may impede accurate parameterization using the BC and vG equations.

The BC-vG Upscaler program was developed by Cheng et al. (2013) to upscale capillary pressure–saturation functions based on a midpoint RPE. Its purpose is to accurately predict average drainage behavior as described by the vG equation at the laboratory column or soil horizon scale based on capillary pressure–saturation data obtained at a physical point and parameterized with the BC equation. In this study, we evaluated and expanded the capability of the BC-vG Upscaler program. Our main objectives were to validate the BC-vG Upscaler with independently measured height-averaged capillary pressure–saturation functions for packed homogeneous sand columns with different heights and to evaluate the impact of using top, middle, and bottom RPEs on the resulting predictions.

Theory

The capillary pressure–saturation function can be measured directly at a physical point using methods such as time domain reflectometry (Sakaki and Illangasekare, 2007) and neutron imaging (Kang et al., 2014). It can also be determined by inverse modeling of water content (averaged across the column height) vs. capillary pressure data obtained using the hanging water column, pressure cell, and centrifuge methods (Jalbert et al., 1999; Dane and Hopmans, 2002; Cropper et al., 2011).

Measured point capillary pressure–saturation functions tend to exhibit a distinct air-entry capillary pressure head (Sakaki and Illangasekare, 2007; Cheng et al., 2013). This is because fewer and shorter interconnected pore networks control air entry as the soil height is reduced. Thus, point functions are best parameterized using the BC equation, which has a pronounced break in slope at this value (Brooks and Corey, 1964):

$$\theta = \theta_s \qquad h \le h_b \tag{1a}$$

$$\theta = \theta_r + (\theta_s - \theta_r)\left(\frac{h_b}{h}\right)^{\lambda} \qquad h > h_b \tag{1b}$$

where θ is volumetric water content, θ_s is saturated volumetric water content, θ_r is residual volumetric water content, h is capillary pressure head, h_b is air-entry capillary pressure head, and λ is the pore-size distribution index.

Cheng et al. (2013) introduced the BC-vG Upscaler program to predict the average capillary pressure–saturation function for a homogenous porous medium of a given height. The BC-vG Upscaler is based on the Liu and Dane (1995) equation relating the average volumetric water content, $\overline{\theta}$, to the height, z_c, and the point BC parameters for the porous medium:

$$\begin{aligned}\overline{\theta} &= \frac{1}{z_c}\int_0^{z_c} \theta(h)\,\mathrm{d}z \\ &= \frac{z^*}{z_c}\theta_s + \frac{z_c - z^*}{z_c}\theta_r + \frac{\theta_s - \theta_r}{z_c} h_b^{\lambda} f(h_{\mathrm{ref}})\end{aligned} \tag{2}$$

where h_{ref} is a reference capillary pressure head measured at elevation z_w, $z^* = 0$ when $(z_w + h_b - h_{\mathrm{ref}}) \le 0$, else $z^* = \min[z_c, (z_w + h_b - h_{\mathrm{ref}})]$, and

$$f(h_{\mathrm{ref}}) = \ln\frac{-z_w + z_c + h_{\mathrm{ref}}}{-z_w + z^* + h_{\mathrm{ref}}}$$

when $\lambda = 1$, else

$$f(h_{\mathrm{ref}}) = \frac{1}{1-\lambda}\left[(-z_w + z_c + h_{\mathrm{ref}})^{1-\lambda} - (-z_w + z^* + h_{\mathrm{ref}})^{1-\lambda}\right]$$

Equation [2] assumes the density of the non-wetting fluid (air) is significantly less than the density of the wetting fluid (water). In developing the BC-vG Upscaler, Cheng et al. (2013) fixed the RPE of the wetting fluid as the midpoint of the porous medium (i.e., $z_w = z_c/2$). This was done to permit comparison with experimental data, which are commonly reported using a midpoint RPE (e.g., Liu and Dane, 1995; Sakaki and Illangasekare, 2007). Equation [2] was then implemented in a forward manner to predict height-averaged capillary pressure–saturation functions.

Unlike θ in Eq. [1], $\overline{\theta}$ in Eq. [2] no longer exhibits a sharp break at the air-entry capillary pressure head. Instead Eq. [2] predicts a smoothed relationship reminiscent of the vG equation (van Genuchten, 1980):

$$\overline{\theta} = \theta_r + (\theta_s - \theta_r)\left[1 + \alpha(h_{\mathrm{ref}})^n\right]^{-m} \tag{3}$$

where α, n, and m are empirical fitting parameters. In the BC-vG Upscaler, Eq. [3] is fitted to the predicted average capillary–pressure saturation functions, yielding inverse estimates of the vG parameters for any height of the porous medium of interest.

The height-averaged water content reflects the drainage of water from the top to the bottom of a packed column or soil layer. As a result, saturation starts to decrease as soon as the top surface of the column drains. For a midpoint RPE, however, the porous medium initially remains fully saturated. This phenomenon becomes more and more pronounced as the height of the column or soil layer increases. Thus, it is necessary to evaluate the performance of the BC-vG Upscaler program using different RPE options.

Materials and Methods

Hanging Water Column Experiments

A coarse homogeneous porous medium, Flint sand (Flint no. 13, U.S. Silica Co.), was selected for use due to its relatively rapid pressure equilibrium times across the range of column lengths studied. The material is mainly composed of quartz (99.8%), with a particle density of 2.65×10^3 kg m^{-3} (Kang et al., 2014). Its grain diameters range from 0.11 to 0.60 mm, with a median grain diameter of 0.56 mm (Kang et al., 2014). The saturated hydraulic conductivity was measured by Kang et al. (2014) on replicate columns of 5.6 ($\pm$0.1) cm height, packed to an average bulk density of 1740 ($\pm$30) kg m^{-3}, using the constant-head method. The resulting average saturated hydraulic conductivity was $1.66 \pm 0.32 \times 10^{-4}$ m s^{-1} (Kang et al., 2014). This value was assumed to be independent of column height.

The Flint sand was packed to different heights in columns of clear polyvinyl chloride pipe with an inner diameter of 1.83 cm. Each column was connected with Tygon tubing, via an outlet at its base, to a burette filled with water (Fig. 1). A high-accuracy pressure transducer (PX409USB, Omega Engineering) was attached to the base of the burette to record cumulative water outflow from the sand column. The measurement was taken at regular time intervals ranging from 1 to 30 s. The inlet at the base of each column was covered with four layers of moist filter paper (Whatman no. 4) to provide a phase barrier.

Each column was partially filled with water, and any air bubbles in the connecting Tygon tubing were removed. Oven-dry Flint sand was then incrementally added to the water in the column in ~4-cm layers until the sand column reached the desired height. During the wet packing process, the column was periodically tapped slightly to minimize air entrapment. The packed sand columns were fully saturated with water by raising the water level in the burette to a height equal to the top of the sand pack, or slightly higher, and then allowed to equilibrate overnight prior to drainage.

At the beginning of each drainage (or hanging water column) experiment, the fully saturated sand columns were clamped to a stationary stand (Fig. 1). The sand columns were then drained stepwise by lowering the burette on the stand. Pressure head steps were typically ~3 cm, but were increased up to ~15 cm if low water outflow indicated that residual saturation was being approached. After each step, and at intervals between steps, the water level in the hanging water column burette, the volume of water in the burette, and the transducer outflow reading were recorded and later used to construct the primary drainage curve. A real-time graphical display of outflow reported by the pressure transducer was used to judge when quasi-equilibrium conditions had been reached for each incremental change in pressure head. Drainage continued in this manner for each column until air passed the phase barrier. After the drainage experiment was complete, the sand was removed from the column, oven dried for 24 h at 105°C, and weighed for bulk density calculations. The porosity was determined based on the measured bulk density values and the known particle density.

Using the protocol described above, a total of 11 drainage experiments were performed on packed columns of Flint sand. Because air passed the phase barrier prior to reaching residual saturation in three of the drainage experiments (Table 1), only 8 of the 11 resulting data sets were used for further analysis. Additionally, drainage data for a 4.3-cm-high column of Flint sand, collected by Kang (unpublished data, 2013) using the same hanging water column method, were included, giving a total of nine experimental data sets. The heights of these nine columns ranged from 4.3 to 55.0 cm (Table 1).

Table 1 contains the measured bulk density, porosity, and minimum (residual) volumetric water content values for each column. All three variables were independent of the column height, as is to be expected. The mean bulk density of the packed columns was 1719 kg m^{-3}, with a coefficient of variation (CV) of only 3.89%. The mean porosity was 0.35 m^3 m^{-3}, with a CV of 7.17%. The minimum (residual)

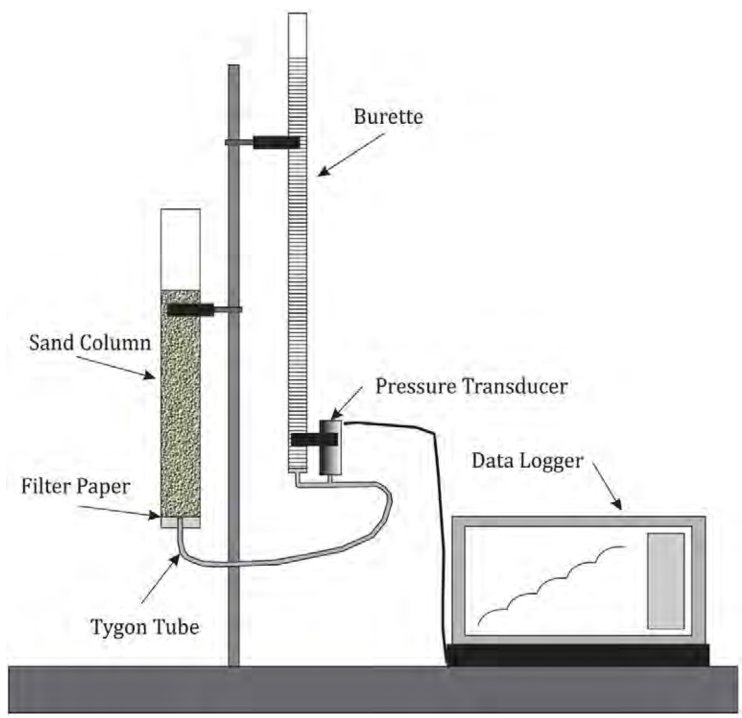

Fig. 1. Hanging water column setup showing sand column, burette, pressure transducer, and data logging computer (adapted from Cropper et al., 2017).

Table 1. Physical properties used to determine effective saturation for Flint sand hanging water column experiments.

Column height	Run no.	Bulk density	Porosity	Minimum (residual) water content
cm		kg m^{-3}	——— m^3 m^{-3} ———	
4.3	R0	1740	0.344	0.040
14.4	R7	1780	0.327	0.046
19.7	R10	1780	0.327	0.021
23.8	R5†	1680	0.367	0.056
24.5	R1†	‡	‡	‡
24.9	R11	1750	0.339	0.054
25.1	R2†	1620	0.389	0.048
29.5	R3	1650	0.377	0.039
37.0	R4	1630	0.385	0.049
43.3	R8	1780	0.327	0.036
48.5	R6	1740	0.343	0.041
55.0	R9	1780	0.329	0.032

† Incomplete data set due to air penetrating the phase barrier prior to reaching residual saturation.
‡ Not measured.

volumetric water content was 0.042 m^3 m^{-3}, with a CV of 24.19%. The CV for this variable was higher than for the other variables in Table 1 because the mean value was close to zero.

Parameterization of Hanging Water Column Data

The average capillary pressure–saturation data from the hanging water column experiments were fitted using the "constrained" form of the van Genuchten (1980) equation, with m replaced by 1 – 1/n:

$$\bar{S}_e = \frac{\bar{\theta} - \theta_r}{\theta_s - \theta_r} = \left[1 + \alpha\left(h_{ref}\right)^n\right]^{-(1-1/n)} \qquad [4]$$

where $\bar{S}_e$ is the average effective saturation. The $\bar{S}_e$ was calculated from the measured average volumetric water contents, $\bar{\theta}$, using porosity for the saturated volumetric water content, θ_s, and minimum volumetric water content for the residual volumetric water content, θ_r. The measured values for porosity and minimum volumetric water content for each column are given in Table 1.

Choosing a midpoint reference capillary pressure head, corresponding to the $z_w = z_c/2$ condition used in the BC-vG Upscaler, produced both positive and negative values for the capillary pressure head during the early stages of drainage. Equation [4] cannot be fitted to data sets containing both positive and negative values of h_{ref}. Thus, data pairs with negative values of h_{ref} would need to be excluded from the fitting. Rather than exclude perfectly good data, the top of the column (i.e., $z_w = z_c$) was selected as the location of the reference capillary pressure head. This resulted in all positive values for h_{ref}. The α and n vG parameters were then estimated by fitting Eq. [4] to the data using nonlinear regression analysis (Marquardt method) in SAS 9.4 (SAS Institute, 2012). All of the fits converged successfully according to the software default convergence criterion. The goodness of fit was assessed based on the root mean square error (RMSE).

Point Capillary Pressure–Saturation Data and Parameterization

Kang et al. (2014) conducted a hanging water column experiment on a 5.6-cm-tall column (with an inner diameter of 1.83 cm) in conjunction with neutron radiographic imaging to characterize the point drainage behavior of Flint sand. The resulting neutron radiographic water content data were processed into a spatial grid of 120 point locations for each of nine imposed quasi-equilibrium basal capillary pressure heads. The capillary pressure heads for the grid locations ranged between 2.66 and 51.73 cm.

For the present study, the Kang et al. (2014) data set was converted to point effective saturation–capillary pressure head data pairs. The point effective saturation, S_e, was calculated, using the maximum observed water content as the saturated volumetric water content, θ_s, and the minimum observed water content as the residual volumetric water content, θ_r, using

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} \qquad [5]$$

The maximum volumetric water content (0.391 m^3 m^{-3}) was determined by arithmetic averaging of the eight observed water contents at the minimum capillary pressure head (2.66 cm). The minimum volumetric water content (0.018 m^3 m^{-3}) was determined by arithmetic averaging of the eight observed water contents at the maximum capillary pressure head (51.73 cm).

The resulting point effective saturation–capillary pressure head values were parameterized by fitting the Brooks and Corey (1964) equation to all 1080 data pairs to produce a composite point water retention function for Flint sand. The BC equation was fitted in the following form:

$$S_e = 1 \qquad h \le h_b \qquad [6a]$$

$$S_e = \left(\frac{h_b}{h}\right)^{\lambda} \qquad h > h_b \qquad [6b]$$

using segmented nonlinear regression analysis (Marquardt method) in SAS 9.4 (SAS Institute, 2012). The fitting procedure converged successfully according to the software default convergence criterion, and the resulting RMSE was 4.33 × 10^{-2}. The BC parameter estimates produced by the nonlinear regression analysis (h_b = 16.93 cm and λ = 5.67) were then used as inputs to the BC-vG Upscaler to predict the average effective saturation as a function of column height.

Forward Prediction of Average Functions

The BC-vG Upscaler program (Cheng et al., 2013), which represents a forward implementation of the approach of Liu and Dane (1995), was used to predict the average effective saturation–capillary pressure head functions for each column. The point BC parameters produced by parameterization of the neutron radiography data of Kang et al. (2014), along with the column heights, were the input parameters. The algorithm generates 120 reference capillary pressure head values ranging between $h_b \times 10^{-2}$ and $h_b \times 10^4$ cm spaced logarithmically to intensely cover the most rapid drainage portion of the water retention curve immediately following air entry (Fig. 2). The software assumes that the elevation of the reference capillary pressure head for the wetting fluid is the midpoint of the column, i.e., $z_w = z_c/2$. It then predicts an average effective saturation value for each generated h_{ref} value using Eq. [2].

To investigate how the RPE position affects the average effective saturation values, the BC-vG Upscaler algorithm was modified so that predictions could also be made for RPEs corresponding to the top, $z_w = 0$, and bottom, $z_w = z_c$, of the columns. Each generated retention data set of 120 data pairs was parameterized by fitting Eq. [4] with the $m = 1 - 1/n$ fitting option selected in the BC-vG Upscaler (Fig. 2).

Results

Forward Prediction of Average Functions

Figure 3 shows the effect of the choice of the RPE on the predicted average volumetric water content–capillary pressure head function for each column used in this study. The curves represent the raw predictions from Eq. [2] before fitting Eq. [4]. For the two shortest column heights (4.3 and 14.4 cm), the volumetric water contents at saturation ($h_{ref} = 0$) agreed for all three RPEs, although there were small differences in the predicted drainage behavior. While the shortest columns produced full drainage data sets for any RPE, column heights greater than these failed to produce complete data sets (i.e., volumetric water contents at saturation less than the porosity at $h_{ref} = 0$) when the bottom RPE was selected. Columns shorter than 37.0 cm produced full drainage data sets for the middle RPE, but taller columns did not. Only the top RPE yielded a complete drainage function for each column.

The impact of parameterizing incomplete data sets can be comprehended by examining the predicted drainage functions for the tallest columns in Fig. 3. The bottom and middle RPE predictions for these columns lack any retention data pairs with average volumetric water contents approaching the porosity. Fitting Eq. [4] to such data sets

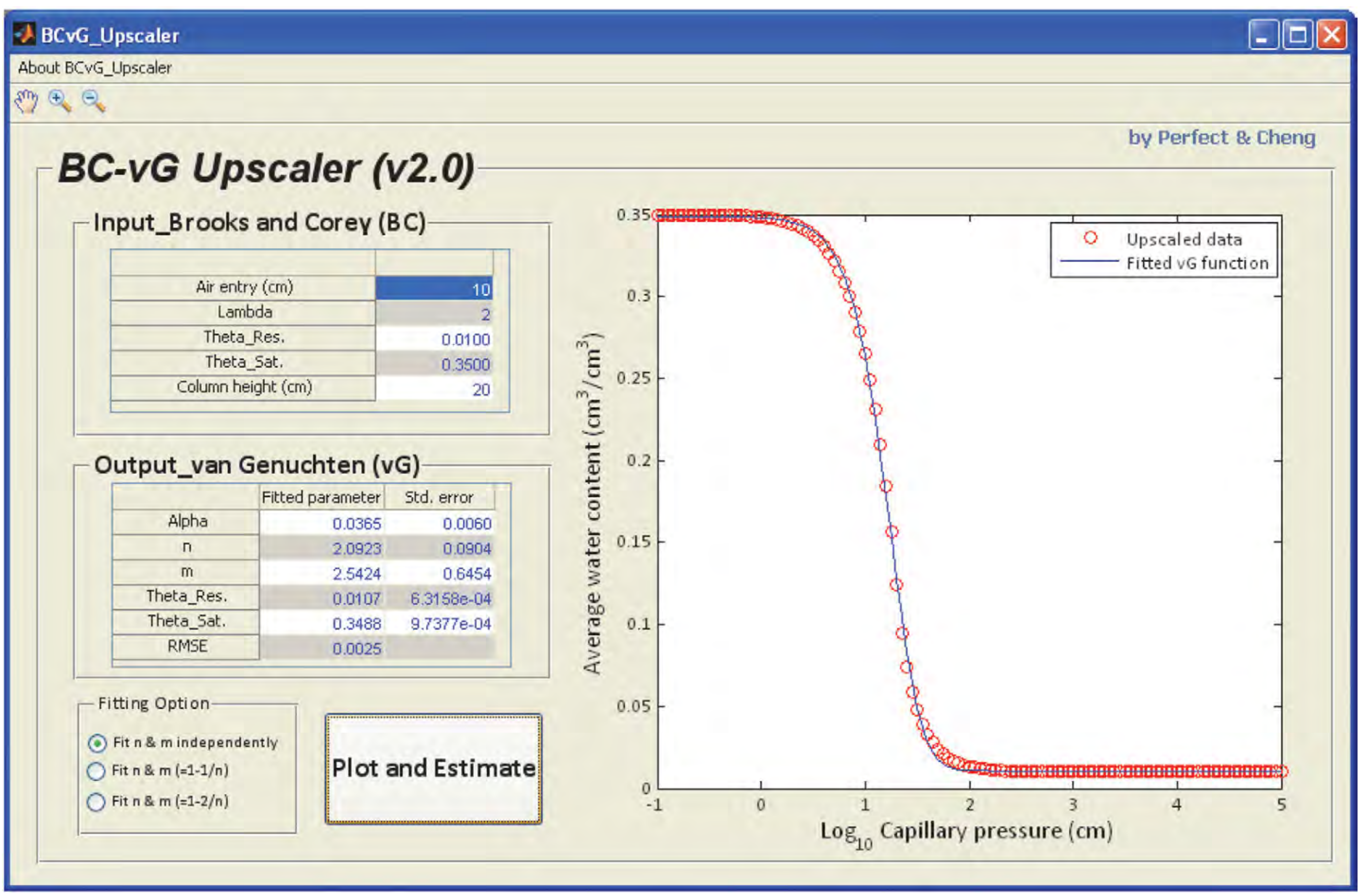

Fig. 2. Screen capture image of the BC-vG Upscaler, showing an example of a height-averaged capillary pressure–saturation function with point Brooks and Corey parameters as the input and average van Genuchten parameters with n and m fitted independently as the output for a column height of 20 cm (adapted from Cheng et al., 2013).

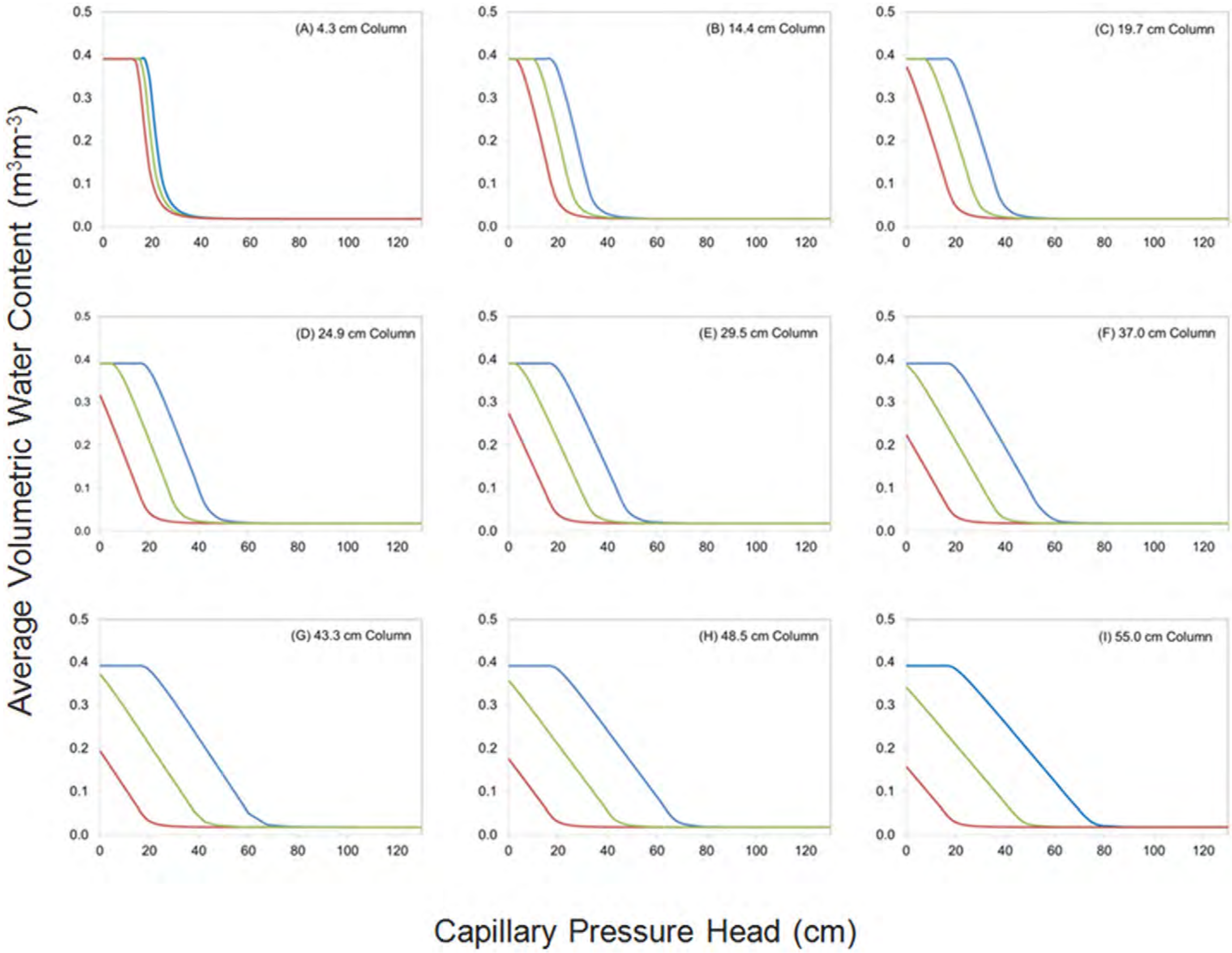

Fig. 3. Comparison of the choice of bottom (red), middle (green), and top (blue) reference pressure elevations in Eq. [2] on predicted average volumetric water content–capillary pressure head functions for nine columns of Flint sand with different heights ranging from (A) 4.3 cm through (I) 55.0 cm.

in the BC-vG Upscaler will invariably lead to inaccurate parameter estimates and incorrect conclusions regarding drainage behavior. This can be seen in Fig. 4 by comparing the predicted drainage curves using the default midpoint RPE in the BC-vG Upscaler with the top RPE predictions and the observed data. The resulting inaccuracies are most apparent for the tallest columns.

Hanging Water Column Data and Parameterization

The nine columns analyzed contained at a minimum 15, and as many as 25, effective saturation–capillary pressure data pairs measured under quasi-equilibrium conditions. Total drainage durations ranged from ~5 h for the 4.3-cm column to ~300 h for the 55.0-cm column. Based on the top reference pressure location, the measured data pairs for each column are shown as black points in Fig. 4.

Equation [4] was fitted to the measured data pairs for each column, yielding the average vG parameters summarized in Table 2. As can be seen in Fig. 4, all of the fits were very good, resulting in the relatively low RMSE values and small parameter standard errors in Table 2. Estimates of the two average vG parameters, α and n, ranged from 0.023 to 0.046 cm^{-1} and from 4.824 to 11.725, respectively. There was a clear dependence of the magnitudes of both parameters on the column height.

Comparison of Observed and Predicted Average Functions

Figure 4 also includes upscaled predicted functions based on the top and midpoint RPEs. In general, the top RPE predictions were in excellent agreement with the observed drainage data and their best-fit vG functions. Effective saturation was systematically overpredicted in three of the columns (19.7, 29.5, and 37.5 cm) and systematically underpredicted in one column (14.4 cm). However, these discrepancies were relatively minor, and the upscaled predictions were very accurate for the majority of the columns (Fig. 4). In comparison, the default midpoint RPE

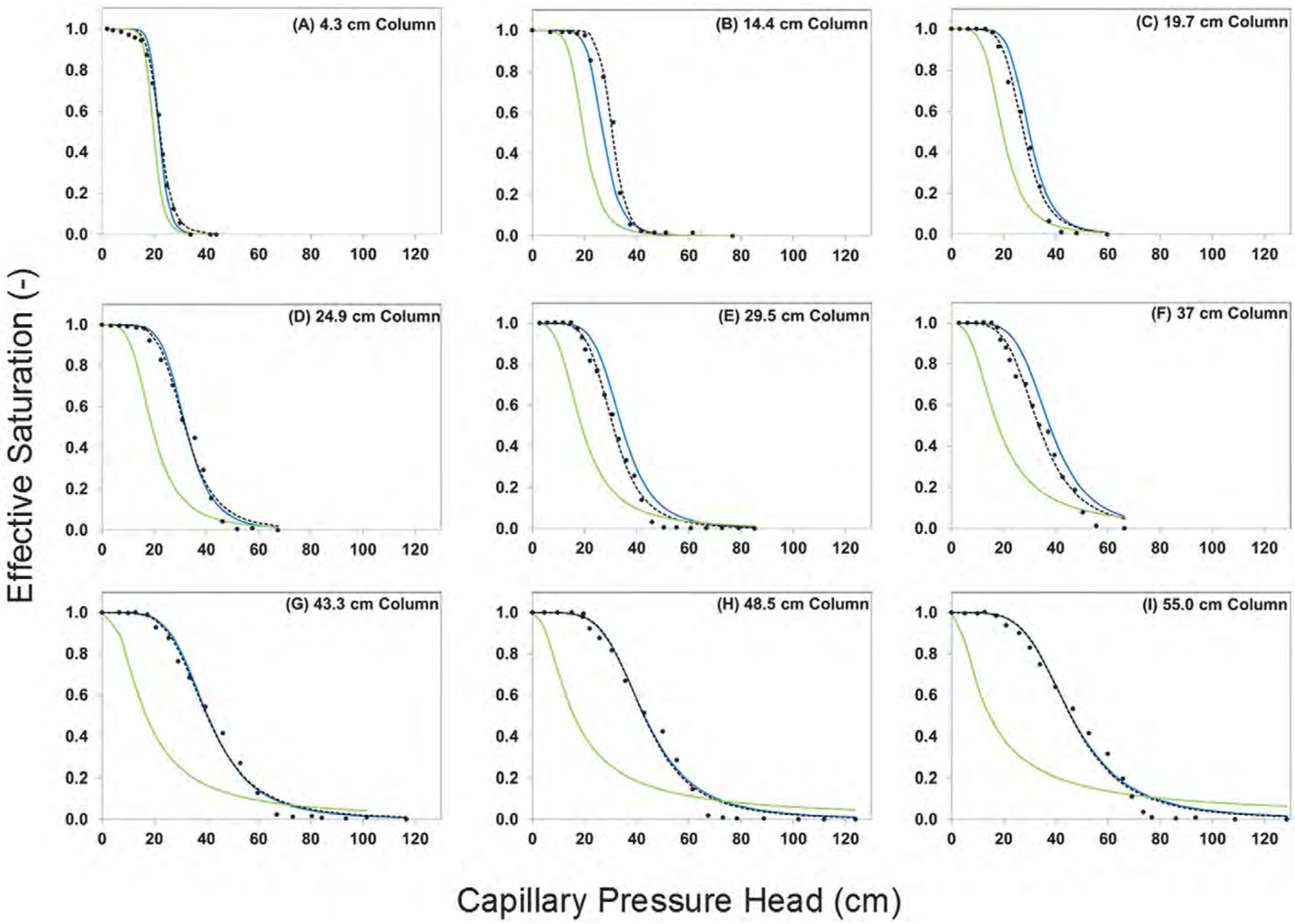

Fig. 4. Upscaled top (solid blue lines) and midpoint (solid green lines) reference pressure elevation predictions of capillary pressure–effective saturation functions compared with measured average data points (black circles) and van Genuchten (1980) functions fitted to measured average data points (dashed black lines) for Flint sand packed into nine columns with different heights ranging from (A) 4.3 cm through (I) 55.0 cm.

in the BC-vG Upscaler resulted in highly inaccurate predictions for the tallest columns.

To evaluate the overall performance of the BC-vG Upscaler using the top RPE, observed effective saturation values for all of the imposed capillary pressure heads, in all nine columns, were linearly regressed against the corresponding predicted effective saturation values. The resulting best fit model (slope = 0.98; intercept = 0.03; $R^2 = 0.98$) corresponded closely to an ideal 1:1 relationship, confirming the good agreement observed for the individual columns in Fig. 4.

The average vG parameter estimates and RMSE statistics produced by upscaling the point BC parameters using the BC-vG Upscaler with the top RPE are given in Table 3. The α and n parameters predicted by the upscaling procedure covered similar ranges of values as those obtained by fitting the observed data (compare the parameter estimates in Table 3 with those in Table 2). For both parameters, the largest and smallest estimates were obtained with the shortest and tallest columns, respectively.

Table 2. Summary of van Genuchten (1980) equation parameters inversely estimated from the measured average effective saturation–capillary pressure data for each Flint sand column.

Column height	Run no.	α	n	RMSE
cm		cm^{-1}		
4.3	R0	0.046 (0.000)†	9.133 (0.453)	2.09×10^{-2}
14.4	R7	0.033 (0.000)	11.725 (1.379)	4.24×10^{-2}
19.7	R10	0.038 (0.001)	6.725 (0.542)	3.87×10^{-2}
24.9	R11	0.033 (0.001)	5.939 (0.456)	4.18×10^{-2}
29.5	R3	0.034 (0.000)	5.915 (0.263)	3.08×10^{-2}
37.0	R4	0.032 (0.000)	5.028 (0.300)	4.24×10^{-2}
43.3	R8	0.027 (0.000)	4.951 (0.274)	3.46×10^{-2}
48.5	R6	0.025 (0.000)	5.129 (0.337)	4.16×10^{-2}
55.0	R9	0.023 (0.000)	4.824 (0.318)	4.50×10^{-2}

† Standard errors in parentheses.

Table 3. Summary of van Genuchten (1980) equation parameters predicted by the BC-vG Upscaler algorithm based on Brooks and Corey point parameters, column height, and a top reference pressure elevation.

Column height	Run no.	α	n	RMSE
cm		cm^{-1}		
4.3	R0	0.046 (0.000)†	12.065 (0.238)	7.98×10^{-3}
14.4	R7	0.038 (0.000)	8.526 (0.083)	4.87×10^{-3}
19.7	R10	0.035 (0.000)	7.418 (0.103)	7.48×10^{-3}
24.9	R11	0.032 (0.000)	6.649 (0.109)	9.44×10^{-3}
29.5	R3	0.030 (0.000)	6.146 (0.111)	1.09×10^{-2}
37.0	R4	0.028 (0.000)	5.542 (0.109)	1.27×10^{-2}
43.3	R8	0.026 (0.000)	5.182 (0.108)	1.40×10^{-2}
48.5	R6	0.025 (0.000)	4.949 (0.108)	1.51×10^{-2}
55.0	R9	0.024 (0.000)	4.704 (0.105)	1.61×10^{-2}

† Standard errors in parentheses.

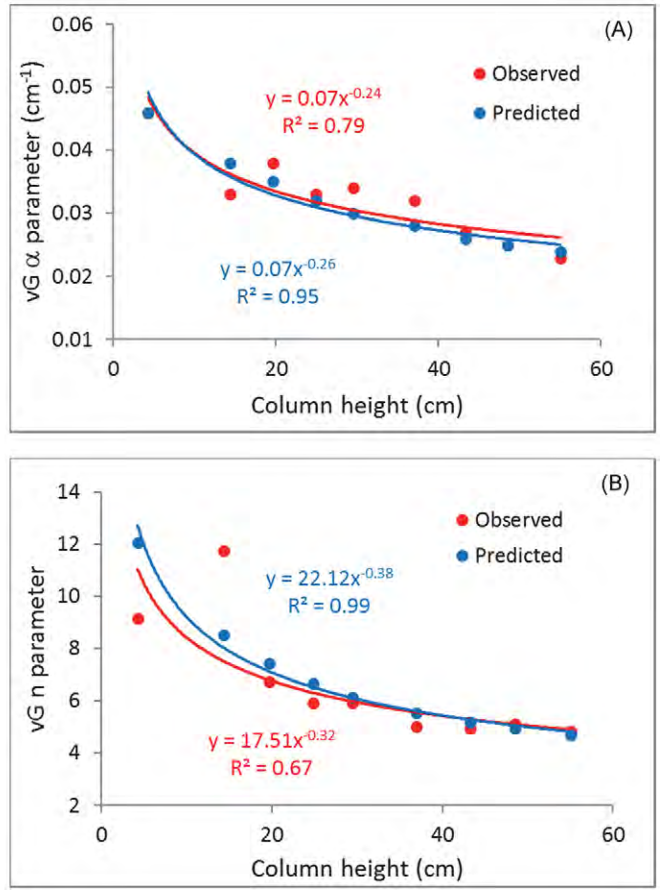

Fig. 5. Column height dependencies of the (A) α and (B) n parameters in the van Genuchten (1980) effective saturation–capillary pressure head equation predicted by the BC-vG Upscaler and fitted to the observed average drainage data. In both cases, a top reference pressure elevation was used.

Figure 5 compares the observed and predicted average van Genuchten (1980) parameters in relation to column height. Both α and n showed a log–log (power model) dependence on column height, with increasing column height resulting in decreasing values of these parameters. The power model explained >95% of the variance in the predicted vG parameters and between 67 and 79% of the variance in the observed vG parameters. The lower R^2 values for the observed parameter models can be attributed to experimental variation among the nine hanging water column data sets, whereas the predicted parameter models were based on upscaled predictions from a single column. Despite these differences in variability, the dependence of the observed and predicted average vG parameters on column height was remarkably similar, as can be seen in Fig. 5. These curvilinear relationships indicate a clear scale dependency in the shape of the average capillary pressure–saturation function.

To further evaluate the performance of the BC-vG Upscaler using the top RPE, the predicted average vG parameter estimates were linearly regressed against the corresponding observed values. The resulting best-fit models corresponded closely to ideal 1:1 relationships for both α (slope = 0.96; intercept = 0.00; $R^2 = 0.87$) and n (slope = 0.77; intercept = 1.73; $R^2 = 0.60$), indicating good statistical agreement between the average vG parameters predicted by the BC-vG Upscaler and the independently estimated parameters.

Discussion and Conclusions

The importance of the choice of the RPE demonstrated in the present study illustrates some of the challenges for experimental measurement of capillary pressure–saturation data. During a monotonic drainage experiment, air (the non-wetting phase) replaces water (the wetting phase) from the top of the column, resulting in variable saturation as a function of elevation. In soil physics, the middle of the column is widely accepted as the RPE for constructing the average capillary pressure–saturation function (e.g., Liu and Dane, 1995; Sakaki and Illangasekare, 2007). This is because column heights in the laboratory are typically <10 cm, and when a column is relatively short, there is little difference between the capillary pressure heads computed using the top, middle, and bottom reference elevations (Liu and Dane, 1995; Sakaki and Illangasekare, 2007; this study). However, short columns often underrepresent the full range of physicochemical conditions in a particular soil horizon and thus may not constitute a representative elementary volume. When column height is increased to address this issue, the shift in the capillary pressure head with reference elevation becomes increasingly significant. The impact of this shift can be clearly seen in Fig. 3. For tall columns, the main consequence is a sequential loss of data pairs (due to negative capillary pressure values) close to saturation. This results in inaccurate parameter estimates when fitting the average vG equation, Eq. [4], to the incomplete data sets.

To avoid inaccurate parameterization of capillary pressure–saturation functions for tall columns, we recommend that the reference elevation for capillary pressure be established as the top of the column for monotonic drainage experiments. Likewise, for monotonic wetting experiments, it seems logical to choose the bottom of the column as the RPE. Wetting experiments with different column lengths should be conducted to verify this second recommendation. Additionally, consideration will need to be given to the most appropriate RPE for tall columns used to investigate hysteresis, in which multiple scanning loops are measured between the primary wetting and drying branches.

Although this investigation has produced strong support for forward modeling with the BC-vG Upscaler, the predictions were based on point parameters for a single column. In future investigations of a similar nature, it would be desirable to determine point parameters on multiple columns. Such an approach would facilitate calculations of the errors associated with the predicted average retention functions for different column heights. It should also be noted that the BC-vG Upscaler is designed to model the heterogeneous distribution of water within a texturally homogeneous material. Further research will be needed to extend this approach to more heterogeneous porous media.

Based on the observations from this study, the BC-vG Upscaler is being updated with an option for selecting different RPEs (i.e., top, midpoint, or bottom) to facilitate the improved prediction of average hydraulic parameters for drainage or wetting curves. It is available free of charge on request to the authors.

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