Forward Prediction of Height-Averaged Capillary Pressure–Saturation Parameters Using the BC-vG Upscaler

There is ongoing interest in approaches for upscaling point (e.g., pixel or voxel scale) measurements of soil hydraulic properties to predict column-scale behavior in the laboratory, or even field-scale processes. We have developed the BC-vG Upscaler for estimating the height-averaged capillary pressure–saturation relationship, $h(h)$, for a given porous medium based on equations used in the TrueCell program. Whereas TrueCell inversely estimates point Brooks and Corey (BC) equation parameters from $h(h)$ data, the BC-vG Upscaler uses point BC parameters as inputs for the forward prediction of height-averaged van Genuchten (vG) parameters. The BC-vG Upscaler was verified using previously published, independent point and height-averaged capillary pressure–saturation data sets for silica sand. The capability of the BC-vG Upscaler was demonstrated in three separate applications. The first showed how the program can be used to predict height-averaged vG equation parameters using three different relationships between $n$ and $m$. The second explored the effects of varying column height on the predicted vG parameters for a hypothetical porous medium. The third used the BC-vG Upscaler to predict height-averaged vG parameters for a 50-cm-tall column based on previously published point BC parameters for a wide range of porous media. The BC-vG Upscaler is available free upon request. It should prove useful for converting point BC parameters into height-averaged vG parameters suitable for inclusion in numerical models for simulating variably saturated flow. The program could also be used to develop new scale-dependent relationships between the parameters of the BC and vG equations.

Abbreviations: BC, Brooks and Corey; GB, glass beads; HL, Hanford sand; LCL, lower coarse layer; MFL, medium fine layer; TDR, time domain reflectometry; UCL, upper coarse layer; vG, van Genuchten.

Because of the scale dependency of many soil hydraulic properties, there is intense and enduring interest in approaches for upscaling measurements obtained at a physical point (e.g., pixel or voxel) to predict column-scale behavior in the laboratory or on small-scale laboratory columns to predict field-scale processes. Vereecken et al. (2007) provided a comprehensive literature review of the different methods that have been used to upscale soil water properties and processes. They distinguished between two basic approaches to upsampling: inverse methods for estimating effective parameters from the application of small-scale constitutive equations to large-scale data sets and forward methods for predicting large-scale parameters from the analysis of small-scale measurements and constitutive equations.

Our specific interest is in upscaling the point capillary pressure–saturation relationship, $\theta(h)$, for a given porous medium, using forward methods. Most previous upscaling studies of this hydraulic property have focused on the prediction of large-scale parameters for heterogeneous porous media with spatially variable $\theta(h)$ relations (e.g., Desbarats, 1995; Green et al., 1996; Zhu et al., 2004). However, differences in scale (specifically height) within the vadose zone can introduce variability in the water content of even a homogenous porous medium simply through their contributions to the local pressure state of the water.

Volume (or height) averaging is a powerful forward upscaling technique that can be used to predict the scale dependency of hydraulic parameters for both homogenous and heterogeneous systems. Quintard and Whitaker (1988) and Ahmadi and Quintard (1996) first introduced the volume averaging approach to predict large-scale capillary pressure–saturation relations for multiphase flow in oil and gas reservoirs. In an experimental study, Bottero et al. (2011) investigated the applicability of various averaging operators for computing...
an average, or upscaled, capillary pressure–saturation curve from small-scale measurements. Liu and Dane (1995a) derived analytical expressions, based on height averaging, for predicting large-scale capillary pressure–saturation functions from the Brooks and Corey (1964) (BC) equation parameters for a physical point in a homogenous porous medium. Rather than using these expressions for forward prediction, however, they developed a computer program (TrueCell) for the inverse estimation of point hydraulic parameters from large-scale data (Liu and Dane, 1995b).

We introduce here a new computer program (the BC-vG Upscaler) that uses the Liu and Dane (1995a) approach in a forward manner and then parameterizes the resulting scale-dependent capillary pressure–saturation relations using the van Genuchten (1980) (vG) equation. This leads to new empirical relationships between the parameters of the Brooks and Corey (1964) and van Genuchten (1980) equations. The BC-vG Upscaler can also be used to predict vG equation parameters for column heights that match the vertical grid or node spacing in numerical models for simulating unsaturated flow. We describe the development of the BC-vG Upscaler program, demonstrate its capabilities, and verify its predictions using an independent data set from Sakaki and Illangasekare (2007).

**Materials and Methods**

Theory

The BC equation for the point capillary pressure–saturation relationship is given by

\[ \theta = \theta_s \quad (h \leq h_b) \]  

\[ \theta = \theta_s + (\theta_c - \theta_s) \left( \frac{h}{h_b} \right) \lambda \quad (h > h_b) \]  

where \( \theta \) is volumetric water content \([L^3 L^{-3}]\), \( \theta_s \) is saturated volumetric water content \([L^3 L^{-3}]\), \( \theta_c \) is residual volumetric water content \([L^3 L^{-3}]\), \( h \) is capillary pressure head \([L]\), \( h_b \) is bubbling capillary pressure head \([L]\), and \( \lambda \) is pore-size distribution index (dimensionless). We assume that both \( \theta \) and \( h \) have been measured at a physical point (e.g., voxel) or in the horizontal plane (e.g., time domain reflectometry [TDR] probe).

Assuming the density of the nonwetting fluid (air) is much less than the density of the wetting fluid (water), Liu and Dane (1995a) showed that Eq. [1] can be height averaged to give the following analytical expression:

\[ \bar{\theta} = \frac{1}{\theta_c} \int_0^{h_c} \theta(h) \, dh = \frac{\theta_s - \theta_c}{\theta_c} + \frac{\theta_c - \theta_s}{\theta_c} \left( \frac{h}{h_b} \right) \lambda \left[ \left( \frac{h}{h_b} \right) - 1 \right]^{\lambda-1} \]  

where \( \bar{\theta} \) is height-averaged volumetric water content \([L^3 L^{-3}]\), \( h_c \) is column height \([L]\), \( \bar{h} \) is capillary pressure head measured at \( \frac{h_c}{2} \) \([L]\); \( \bar{z}^* = 0 \) if \( \frac{h}{2} + h_b - \bar{h} \) \( \leq 0 \), else \( \bar{z}^* = \min[\bar{z}_c, (\frac{h_c}{2} + h_b - \bar{h})] \), and \( f(\bar{h}) = \ln((\frac{h_c}{2} + \bar{h})/(\frac{h}{2} + \bar{z}^* + \bar{h})) \) if \( \lambda = 0 \), else \( f(\bar{h}) = 1/(1 - \lambda)[(\frac{h_c}{2} + \bar{h})^{-\lambda} - (\frac{h_c}{2} + \bar{z}^* + \bar{h})^{-\lambda}] \). Unlike \( \theta \) in Eq. [1], \( \bar{\theta} \) in Eq. [2] no longer exhibits a sharp break at the bubbling pressure. Instead, Eq. [2] predicts a smoothed relationship graphically reminiscent of the vG equation:

\[ \bar{\theta} = \theta_s + (\theta_c - \theta_s) \left[ 1 + (\alpha \bar{h})^n \right]^{-m} \]  

where volumetric water content and capillary pressure head are assumed to be averaged quantities and \( \alpha \) \([L^{-1}]\), \( n \) (dimensionless), and \( m \) (dimensionless) are empirical fitting parameters.

Several researchers have derived theoretical relationships between the parameters of the BC and vG equations (e.g., van Genuchten, 1980; Lenhard et al., 1989; Morel-Seytoux et al., 1996; Zhu et al., 2004). However, none of these studies approached the problem by noting the equivalency between Eq. [2] and [3]. Because an analytical solution to the resulting expression has proved elusive, we have developed the BC-vG Upscaler to estimate average vG equation parameters by fitting Eq. [3] to the relationship predicted by Eq. [2] for a given set of BC parameters and column height using nonlinear regression (see below).

**The BC-vG Upscaler**

The BC-vG Upscaler was developed with a graphical user interface (GUI) using the curve-fitting toolbox and GUI development tools under MATLAB (Version 7.11, R2010b, The MathWorks Inc.). Based on the input BC \( h_b \) parameter, the BC-vG Upscaler first generates 120 height-averaged capillary head values \( [\text{cm}] \) using the expression \( \bar{h} = h_b \times 10^{i-1} \), where \( i = -1 \) to 5 in increments of 0.05. The logarithmic spacing was designed to intensively cover the air-entry and rapid-drainage regions of the capillary pressure–saturation curve. Although our choice of the total number of points was somewhat arbitrary, this number has proved to be adequate for the nonlinear fitting. As a refinement, user-specified \( \bar{h} \) values could be implemented in future versions of the BC-vG Upscaler. Based on the generated \( \bar{h} \) values, the input BC equation parameters, and the user-specified column height, Eq. [2] is used to compute 120 \( \bar{\theta} \) values. Equation [3] is then fitted to the resulting \( \bar{\theta}(\bar{h}) \) data set using the nonlinear regression algorithm (nlinfit) provided by the MATLAB curve-fitting toolbox (MathWorks, 2012). The nlinfit algorithm uses the Levenberg–Marquardt nonlinear least squares algorithm (Marquardt, 1963). The input BC equation parameter values are used as the initial guesses for the nonlinear fitting calculations, with \( h_b \) converted to \( \alpha \) using \( \alpha = 1/h_b \) and \( \lambda \) converted to \( n \) and \( m \) using \( n = \lambda + 1 \) and \( m = 1 - 1/(\lambda + 1) \), respectively (van Genuchten, 1980).
Various outputs are produced following model convergence. The graphical output is a plot constructed from the 120 $h_\theta$ values generated using Eq. [2] along with the best-fit vG relationship, Eq. [3], predicted by the parameter estimates from the nlinfit algorithm. These parameter estimates, their associated standard errors, and the root mean square error (RMSE) of the fit are reported in the output vG box. The parameter standard errors are estimated from confidence intervals using the nlinparci function on the Jacobian matrix calculated by nlinfit, while the RMSE is calculated directly from nlinfit. The $n$ and $m$ parameters in Eq. [3] are estimated independently as the default condition. It is also possible to estimate the $n$ parameter with $m$ dependent on $n$, as described by the following commonly used expressions (van Genuchten et al., 1991):

$$m = 1 - \frac{1}{n} \quad [4a]$$

$$m = 1 - \frac{2}{n} \quad [4b]$$

For these cases, the standard errors of $m$, $SE_m$, were estimated as

$$SE_m \approx SE_n \frac{dm}{dn} = \frac{SE_n}{n^2} \quad [5a]$$

$$SE_m \approx 2SE_n \frac{dm}{dn} = \frac{2SE_n}{n^2} \quad [5b]$$

respectively, where $SE_n$ is the standard error of $n$.

Figure 1 shows a screen capture image of the BC-vG Upscaler after fitting one of the example applications discussed below. The box on the upper left contains the input BC equation parameters along with the specified column height. The box on the lower left contains the estimated vG equation parameters associated with these input values, along with their standard errors and the RMSE of the fit. The output values were obtained by filling in the input cells, selecting the fitting option ($n$ and $m$ fitted independently in this case) and clicking on the “Plot and Estimate” button. This process also produces the figure on the right, which enables a visual inspection of the goodness-of-fit. An executable version of the BC-vG Upscaler program can be obtained free of charge on request. The source code is also available on request for advanced users.

The BC-vG Upscaler code was checked by entering the data used to construct the graphical output in Fig. 1 into TrueCell (Liu and Dane, 1995b) and specifying the column height and measurement elevations of the wetting and nonwetting fluids ($= z_c/2$ in Eq. [2]), with $n$ and $m$ fitted independently. Only 99 of the 120 $h_\theta$ values were used because this is the maximum allowable number for input to TrueCell. When the predictions from Eq. [2] were used, TrueCell returned output values of the point BC equation parameters that were the same as those entered as inputs to the BC-vG Upscaler. When data for the best-fit vG relationship predicted using the output vG parameters from the BC-vG Upscaler in Eq. [3] were used, the TrueCell-estimated BC equation parameters deviated by an average of 3.4% from the values that were entered as inputs to the BC-vG Upscaler. The maximum deviation observed was 10% for the $\theta_r$ parameter (i.e., 0.011 vs. 0.010).
Validation

The BC-vG Upscaler was validated against independent capillary pressure–saturation data for silica sand no. 8 from Sakaki and Illangasekare (2007), who simultaneously measured the point and average capillary pressure–saturation functions using a modified Tempe cell (of 10 cm height) with a TDR probe inserted horizontally at a height of 5 cm. (For a detailed description of the experimental setup and methods, see Sakaki and Illangasekare, 2007.)

We fitted Eq. [1] to the measured point (TDR) data using segmented nonlinear regression (Levenberg–Marquardt method; Marquardt, 1963). The RMSE of the fit was 0.005. The resulting BC equation parameters were then entered into the BC-vG Upscaler, along with the column height of 10 cm, to give a forward prediction of the average vG equation parameters. The predicted parameters were compared with vG parameters estimated inversely by fitting Eq. [3] to the measured average (Tempe cell) data, again using the Levenberg–Marquardt nonlinear regression method. The predictions of the two sets of vG parameters were compared statistically using a paired t-test.

Example Applications

We explored three predictive applications to demonstrate the capability of the BC-vG Upscaler. The first of these involved a single set of BC parameters for a hypothetical soil and a single column height. The BC-vG Upscaler was used to estimate vG equation parameters based on three different relationships between \( n \) and \( m \). The second application involved using the BC-vG Upscaler to estimate vG equation parameters for hypothetical soils with different BC parameters and variable column heights. In this example, the relationship between the vG parameters \( n \) and \( m \) was determined by Eq. [4a]. Relations between the vG parameter estimates and column height were then investigated.

The final application involved predicting vG parameters for the different porous media described by Cropper et al. (2011) using a single column height of 50 cm and \( n \) and \( m \) fitted independently. The materials studied were Berea sandstone (a sedimentary rock core), glass beads (45–70-μm diameter, GB), disturbed Hanford sand (HL), and undisturbed sediments from the upper coarse layer (UCL), medium fine layer (MFL), and lower coarse layer (LCL) at the Hanford site. Point BC parameter estimates for these porous media were obtained from Cropper et al. (2011, Tables 1 and 5); in each case, we selected the values for replicate no. 1.

Results and Discussion

The results of fitting Eq. [1] to the point capillary pressure–saturation data for silica sand no. 8 from Sakaki and Illangasekare (2007) are illustrated in Fig. 2. Clearly, the BC equation, with its distinctive break in behavior at \( h_b = 5.877 \) cm, provided an excellent fit to these point measurements. The BC point parameter estimates are given in Table 1. These values were entered into the BC-vG Upscaler to predict the vG equation parameters for a 10-cm-tall column. The results of this exercise are summarized in Table 1, which also includes separate inverse estimates of the vG parameters obtained by fitting Eq. [3] to the average capillary pressure–saturation data for silica sand no. 8 from Sakaki and Illangasekare (2007).

<table>
<thead>
<tr>
<th>Method</th>
<th>Parameter estimates</th>
<th>RMSE</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( \theta_s )</td>
<td>( \theta_r )</td>
</tr>
<tr>
<td>Inverse estimation by fitting height-averaged data</td>
<td>0.387 (0.006)‡</td>
<td>0.015 (0.009)</td>
</tr>
<tr>
<td>Forward prediction from point data (BC-vG Upscaler)</td>
<td>0.392 (0.003)†</td>
<td>0.027 (0.002)</td>
</tr>
</tbody>
</table>

† In both cases, \( n \) and \( m \) were fitted as \( m = 1 - 1/n \).
‡ Standard errors in parentheses.
The RMSE for the forward prediction using the BC-vG Upscaler was lower than that associated with fitting Eq. [3] to the measured average capillary pressure–saturation data (inverse estimation) (Table 1). This difference in RMSE values emphasizes just how closely Eq. [2] is approximated by Eq. [3].

The two sets of vG parameter estimates were very similar (Table 1). Based on their standard errors, there were no significant differences at the 95% confidence level \( P < 0.05 \) between the forward-predicted and inversely estimated values of \( \theta_s, \theta_r, n, \) and \( m \). The \( \alpha \) parameter value predicted by the BC-vG Upscaler, however, was significantly greater than the inverse estimate at \( P < 0.05 \).

Figure 3 shows the predicted vG relationships from the BC-vG Upscaler and the inverse estimation method alongside the average (Tempe cell) capillary pressure–saturation data for silica sand no. 8 from Sakaki and Illangasekare (2007). The experimental data and vG functions exhibit only a gradual decrease in volumetric water content with increasing capillary pressure head across the air-entry region, which contrasts with the sharp break observed with the point measurements and BC function (compare Fig. 2 and 3). As can be seen, both of the predicted vG relationships closely match the curvilinear nature of the average data.

Although individual vG parameters can be compared statistically (as was done above), this is not a particularly robust evaluation of the BC-vG Upscaler. This is because the chance of getting a non-significant difference is enhanced by the number of comparisons that must be made with multiple parameters. Instead it is more desirable to compare the predicted values of \( \theta_s \) associated with each set of vG parameters. Such an assessment compares the integrated effect of all of the parameters in a single test. To do this, we computed predicted values of \( \theta_s \) (corresponding to the 21 measured values of \( \theta_s \)) using the two sets of vG parameters listed in Table 1. A paired \( t \)-test was then performed on these values, resulting in a \( t \)-value of \( -1.06 \), which was not significant at \( P < 0.05 \). Based on this test, we concluded that there was no statistical difference between the vG relationship for silica sand no. 8 predicted from the point BC parameters using the BC-vG Upscaler and that obtained by inversely fitting the average capillary pressure–saturation data.

**Effect of Fitting Method**

The BC-vG Upscaler includes three options for estimating vG equation parameters from point BC equation parameters. These are: (i) fit \( n \) and \( m \) independently (the default), (ii) fit \( n \) and \( m \) using Eq. [4a], and (iii) fit \( n \) and \( m \) using Eq. [4b]. Table 2 summarizes the results of upscaling from a single set of point BC equation parameters to a column height of 20 cm. In this case, all three options were viable, so estimates from the fitting method with the lowest RMSE (Option i) should be selected. In some cases, however, fitting \( n \) and \( m \) independently results in uniqueness problems in the parameter estimation process. This is a common issue encountered with the use of Eq. [3] (van Genuchten et al., 1991). Typically, \( m \) and \( n \) become strongly correlated, leading to poor convergence and ill-defined parameter values with large confidence intervals. When this phenomenon occurs, a message window will pop up warning users that some of the fitted parameters are not well estimated. In this case, one of the other two fitting methods should be selected. In our experience, Eq. [4a] (Option ii) generally gives

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**Table 2. Comparison of van Genuchten equation parameter estimates for a column height of 20 cm predicted from Brooks and Corey point parameters (saturated water content \( \theta_s = 0.35 \) \( \text{m}^3 \text{m}^{-3} \), residual water content \( \theta_r = 0.01 \) \( \text{m}^3 \text{m}^{-3} \), bubbling capillary pressure head \( h_b = 10 \) cm, and pore-size distribution index \( \lambda = 2 \)) with the BC-vG Upscaler using three different relationships between \( m \) and \( n \).**

<table>
<thead>
<tr>
<th>Method</th>
<th>Parameter estimates</th>
<th>( \theta_s ) ( \text{m}^3 \text{m}^{-3} )</th>
<th>( \theta_r ) ( \text{m}^3 \text{m}^{-3} )</th>
<th>( \alpha ) cm (^{-1} )</th>
<th>( n )</th>
<th>( m )</th>
<th>RMSE</th>
</tr>
</thead>
<tbody>
<tr>
<td>( n ) and ( m ) fitted independently</td>
<td>0.349 (9.7 ( \times 10^{-4} ))†</td>
<td>0.011 (6.3 ( \times 10^{-4} ))</td>
<td>0.037 (0.006)</td>
<td>2.092 (0.090)</td>
<td>2.542 (0.645)</td>
<td>0.003</td>
<td></td>
</tr>
<tr>
<td>( n ) and ( m ) fitted with ( m = 1 - 1/n )</td>
<td>0.346 (0.002)</td>
<td>0.009 (0.001)</td>
<td>0.079 (0.002)</td>
<td>3.085 (0.092)</td>
<td>0.676 (0.010)</td>
<td>0.005</td>
<td></td>
</tr>
<tr>
<td>( n ) and ( m ) fitted with ( m = 1 - 2/n )</td>
<td>0.345 (0.002)</td>
<td>0.009 (0.002)</td>
<td>0.091 (0.003)</td>
<td>3.804 (0.111)</td>
<td>0.474 (0.015)</td>
<td>0.006</td>
<td></td>
</tr>
</tbody>
</table>

† Standard errors in parentheses.
a lower RMSE than Eq. [4b] (Option iii), as was the case in Table 2. When upscaling parameters for a range of column heights or different materials, fitting $n$ and $m$ independently might work for some cases but not others. Under such circumstances, it is best to use Option ii for all of the different permutations, even though this approach will result in slightly higher RMSE values for those cases that could have been fitted with $n$ and $m$ treated as independent parameters. This will allow a consistent evaluation of the effects of column height or porous medium on the upscaled vG parameters.

**Effect of Column Height**

Fitting $n$ and $m$ independently did not produce unique solutions for all of the column heights investigated in this application. Therefore, as noted above, the vG equation parameters were determined using the relationship between $n$ and $m$ given by Eq. [4a]. Using this fitting method still resulted in excellent goodness-of-fit as evidenced by the RMSE values, which ranged from 0.002 to 0.007 for the 10 predicted vG functions shown in Fig. 4.

As expected, the predicted vG functions displayed a pronounced dependence on the column height (Fig. 4). As the column height increased, the estimated saturated water content at $h = 0$ cm decreased. Additionally, the sharp change in slope associated with air entry at the bubbling pressure head predicted by the underlying point BC function (10 cm in this case) became increasingly smoothed out. Vogel et al. (2000) have shown that relatively small changes in the shape of the capillary pressure–saturation function in this region can significantly affect the results of numerical simulations of unsaturated flow, including the performance of the numerical scheme itself in terms of stability and rate of convergence. Based on values of $\bar{h}^{-1}$ evaluated at $\max\{\partial \bar{S}/\partial \bar{h}\}$, the calculated pore radius where drainage is most rapid will decrease with increasing column height. Although there is no visible effect of column height on the residual water content as $\bar{h} \rightarrow \infty$ in Fig. 4, inspection of the best-fit estimates for this parameter (see below) indicated significant decreases with increasing column height.

The preceding analyses were repeated for $h_b$ values between 10 and 1000 cm, with $z_c$ ranging between 10 and 10,000 cm. The individual vG parameter estimates generated by the BC-vG Upscaler were then plotted as a function of dimensionless column height ($z_c/h_b$). For small dimensionless column heights, upscaled estimates of the vG saturated and residual volumetric water contents were similar to the corresponding point BC values (Fig. 4 and 6). However, both parameters decreased with increasing dimensionless column height, eventually leveling off well below the input values.

To facilitate comparison with dimensionless column height, the estimated $\alpha$ values were also expressed in dimensionless terms using the expression $\alpha^* = \alpha h_b$. The results are shown in Fig. 7 along with the values predicted using the following expressions:

\[
\alpha^* = 1 \quad \text{(van Genuchten, 1980) [6a]}
\]

\[
\alpha^* = \left\{0.72 - 0.35 \exp\left(-\frac{\lambda}{\alpha^*}ight)\right\}^{1/\lambda}
\times \left\{0.72 - 0.35 \exp\left(-\frac{\lambda}{\alpha^*}\right)\right\}^{\lambda/(1-\lambda)} - 1\right\}^{1/\lambda} \quad \text{(Lenhard et al., 1989) [6b]}
\]
where $p = (3n - 1)/(n - 1)$. It can be seen that the Lenhard et al. (1989) model, Eq. [6b], predictions were quite good for small dimensionless column heights but overestimated the upscaled $\alpha^*$ values at large dimensionless column heights. The predictions of the van Genuchten (1980) model, Eq. [6a], were consistently too high. Only the Morel-Seytout et al. (1996) model, Eq. [6c], was responsive to changes in the dimensionless column height, and this model gave the closest estimates when comparing averages for all of the column heights considered (i.e., $\alpha^* = 0.60$ vs. 0.51 for the upscaled and predicted average values, respectively). It is clear, however, that none of the existing theoretical relationships between $\alpha$ and $h_b$ fully captured the scale dependency exhibited by the BC-vG Upscaler estimates.

Figure 8 shows the upscaled estimates of $n$ as a function of dimensionless column height (column height divided by the bubbling capillary pressure head, $z_c/h_b$) obtained using the BC-vG Upscaler with $m = 1 - 1/n$ and the following input parameters: saturated water content $\theta_s = 0.35$ m$^3$ m$^{-3}$, residual water content $\theta_r = 0.01$ m$^3$ m$^{-3}$, $h_b = 10$ to 1000 cm, pore-size distribution index $\lambda = 2$, and $z_c = 10$ to 10,000 cm. The dashed lines denote the $n$ values predicted by the van Genuchten (1980), Lenhard et al. (1989), and Morel-Seytoux et al. (1996) models.

The $n$ values declined rapidly with increasing dimensionless column height. Neither Eq. [7a] nor [7b] was able to capture this scale dependency. Both expressions overestimated the upscaled vG $n$ parameter for tall columns, although the van Genuchten (1980) and Morel Seytoux et al. (1996) model predictions were generally
much closer (i.e., within 5% of the BC-vG Upscaler estimates when comparing values averaged across all of the dimensionless column heights considered).

Figures 5 to 8 clearly demonstrate the need for further research on the scale dependency of the relationships between the BC and vG equation parameters. They were developed by varying both $h_b$ and $\varepsilon_c$ in the BC-vG Upscaler while holding $\theta_s$, $\theta_r$, and $\lambda$ constant. The BC-vG Upscaler should be a valuable tool for researchers interested in developing similar relationships for a wide range of materials with different $\theta_s$, $\theta_r$, and $\lambda$ values.

**Effect of Porous Medium**

Point BC equation parameters for the Berea sandstone, GB, HL, UCL, MFL, and LCL materials investigated by Cropper et al. (2011) are reproduced in Table 3. This small but diverse group of porous media permits a rigorous evaluation of the BC-vG Upscaler across a broad range of physical conditions, including consolidated (Berea sandstone) vs. unconsolidated (GB, HL, UCL, MFL, and LCL), sieved and repacked (GB and HL) vs. undisturbed (UCL, MFL, and LCL), high porosity (HL with $\theta_s = 0.413$) vs. low porosity (Berea sandstone with $\theta_s = 0.183$), coarse texture (LCL with $h_b = 7.22$ cm) vs. fine texture (GB with $h_b = 75.49$ cm), and wide pore-size distribution (Berea sandstone with $\lambda = 0.827$) vs. narrow pore-size distribution (GB with $\lambda = 4.798$). The BC equation parameters in Table 3 were entered into the BC-vG Upscaler to predict vG $\overline{B}(h)$ parameters for a 50-cm-tall column of each porous medium. The first point to note is that, in contrast to the previous application, fitting $n$ and $m$ independently yielded unique solutions for all of the materials investigated. The results of these fits are summarized in Table 4.

Regardless of the type of porous medium, the BC-vG Upscaler provided an excellent approximation of the $\overline{B}(h)$ relationship predicted by Eq. [2]. This can be seen from the low RMSE values in Table 4, which ranged from $1.7 \times 10^{-4}$ to $3.6 \times 10^{-3}$. As expected, the unconsolidated, undisturbed, coarse-grained materials produced slightly poorer fits (higher RMSE values and larger parameter standard errors) than the other porous media. With the sole exception of the coarse-grained LCL material, the upscaled $\theta_s$ and $\theta_r$ parameters were virtually identical to their corresponding BC inputs. The $\alpha$ values ranged from 0.012 cm$^{-1}$ for GB to 0.025 cm$^{-1}$ for UCL and gave a different ranking from that produced by the input BC $h_b^{-1}$ values. The independent estimates of $n$ and $m$ ranged from 1.554 to 8.574 and 0.098 to 2.867, respectively.

We did not attempt to predict the estimated $\alpha$ and $n$ values from the input BC equation parameters using Eq. [6] and [7], as was done in the previous application. This is because those theoretical expressions were all derived assuming that $n$ is related to $m$ as described by Eq. [4a]. The $n$ and $m$ parameters in Table 4 were all estimated independently. New empirical relationships can be developed by linking the two sets of parameters in Tables 3 and 4. This task and exploration of the interaction between column height and type of material, however, are beyond the scope of this study; we leave them as open questions to be answered by future researchers.

Our purpose has been to introduce the BC-vG Upscaler, verify its predictions, and present some applications that give an idea of its potential. We believe the real value of this program will come...
The capability of the BC-vG Upscaler was demonstrated in three separate applications. The first of these showed how the program can be used to predict height-averaged vG equation parameters using three separate functional relationships between $n$ and $m$. The second application explored the effects of varying column height on the predicted vG equation parameters for hypothetical porous media when $n$ and $m$ are related through Eq. [(4a)]. In the final application, the BC-vG Upscaler was used to predict vG equation parameters for a wide range of porous media from Cropper et al. (2011) using a single column height.

We believe that the BC-vG Upscaler will prove useful to a wide range of researchers interested in the scale dependency of soil hydraulic properties. Numerical models for simulating unsaturated flow require hydraulic parameters to be assigned to the grid blocks or nodes discretizing the porous medium. Because the scale of these grid blocks or nodes can be much greater than the laboratory measurement scale (Desbarats, 1995; Bottero et al., 2011), the BC-vG Upscaler could be used to predict vG equation parameters for column heights that match the vertical grid spacing in numerical models. If only average capillary pressure–saturation data are available for a single column height, TrueCell should be first used to extract the BC equation parameters for a physical point. These parameters can then be used in conjunction with the BC-vG Upscaler to predict vG equation parameters for any column height of interest. The BC-vG Upscaler should also be valuable for testing existing theoretical relationships between the parameters of the BC and vG equations, as well as for developing new relationships (both empirical and theoretical) and exploring their scale dependency. It is available free of charge on request.

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We have developed a program, the BC-vG Upscaler, for the prediction of height-averaged capillary pressure–saturation relations based on the TrueCell program of Liu and Dane (1995a, 1995b). The essential difference between the two approaches is that TrueCell is a program for inversely estimating point BC equation parameters from height-averaged capillary pressure–saturation data, whereas the BC-vG Upscaler uses point BC parameters as inputs for the forward prediction of average vG equation parameters as a function of column height. We have verified the predictions of the BC-vG Upscaler using independent point and height-averaged capillary pressure–saturation data sets for a coarse sand (no. 8) from Sakaki and Illangasekare (2007).

Acknowledgments

Funding for C.-L. Cheng was provided by the Joint Directed Research and Development (JDRD) program of the UT–ORNL Science Alliance at the University of Tennessee-Knoxville and the Laboratory Directed Research and Development (LDRD) program of Oak Ridge National Laboratory (ORNL). Oak Ridge National Laboratory is managed by UT-Battelle, LLC, for the U.S. Department of Energy under Contract No. DE-AC05-00OR22725. We thank Dr. Toshitoh Sakaki for providing the data from Sakaki and Illangasekare (2007) in spreadsheet format.

References