A Simple Extension of Two-Phase Characteristic Curves To Include the Dry Region

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Abstract

Two-phase characteristic curves are necessary for the simulation of water and vapor flow in porous media. Existing functions such as van Genuchten, Brooks and Corey, and Luckner et al. have significant limitations in the dry region as the liquid saturation goes to zero. This region, which is important in a number of applications including liquid and vapor flow and vapor-solid sorption, has been the subject of a number of previous investigations. Most previous studies extended standard capillary pressure curves into the adsorption region to zero water content and required a refitting of the revised curves to the data. In contrast, the present method provides for a simple extension of existing capillary pressure curves without the need to refit the experimental data. Therefore, previous curve fits can be used, and the transition between the existing fit and the relationship in the adsorption region is easily calculated. The data-model comparison shows good agreement. This extension is a simple and convenient way to extend existing curves to the dry region.

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Introduction

Two-phase characteristic curves are essential for the mechanistic calculation of water and vapor flow in the vadose zone by simulation codes. Commonly employed characteristic curve functions include van Genuchten (1980), Brooks and Corey (1966), and Luckner et al. (1989). These equations are relatively simple and seem to fit a wide range of capillary pressure and relative permeability data. However, the functions all have significant limitations at low liquid saturations in that they use a parameter called residual saturation, which is the minimum liquid saturation calculated by these equations. As the liquid saturation approaches the residual value, the capillary pressure approaches infinity as does the slope, while the liquid-phase relative permeability approaches zero. Unfortunately, this behavior of the capillary pressure curve, along with a small but non-zero relative permeability for the liquid phase, causes significant problems in numerical simulators, often causing them to proceed at extremely small time steps or not at all.

In addition to liquid flow, capillary pressure curves are important for the description of vapor flow at low liquid saturations. Vapor diffusion at low liquid saturations is predominantly driven by vapor pressure differences even under nonisothermal conditions (Plumb et al., 1999; Webb, 1999), which are in turn driven by local vapor pressure lowering. Vapor pressure lowering can be related to capillary pressure through Kelvin's equation (Dullien, 1992), so that vapor flow is significantly influenced by the capillary pressure curve at low liquid saturations.

The limitations of the two-phase characteristic curves in the low liquid saturation region leads to errors in liquid and vapor transport and in the prediction of the actual liquid saturation in this region. An area where this value is important is in the transition from liquid-solid sorption to vapor-solid sorption which is typically at four to six monomolecular layers, or a liquid saturation of 0.11 to 0.16 based on a soil surface area of 25 m²/g (Webb et al., 1999). At higher liquid saturations, adsorption is primarily by liquid-solid processes. As the liquid saturation decreases, however, vapor-solid sorption contributes more and more to the adsorption process and may dominate at low values of liquid saturation. Vapor-solid sorption is important for TCE transport in the subsurface (Ong and Lion, 1991; Petersen et al., 1995) and in explosive vapor transport from buried unexploded ordnance and landmines (Webb et al., 1999).

Common *ad hoc* fixes used in numerical simulations to circumvent these limitations include 1) specifying the residual saturation for capillary pressure lower than that for relative permeability, 2) linearization of the capillary pressure curve at an arbitrary liquid saturation slightly greater than the residual value such that the slope of the capillary pressure curve is always finite, and 3) specifying a maximum capillary pressure. While the modifications allow numerical simulations to proceed, they are arbitrary, and a better and more meaningful modification is needed.

Physically-based modification of the capillary pressure curve has been suggested by a number of authors recently, including Ross et al. (1991), Campbell and Shiozawa (1992), Rossi and Nimmo (1994), Fayer and Simmons (1995), and Morel-Seytoux and Nimmo

(1999). Ross (1991) modified the Campbell (1974) water retention function to match oven dry conditions without changing the basic equation; the equation parameters were simply refit to the data. Campbell and Shiozawa (1992) obtained dry region capillary pressure data and made the interesting observation that the capillary pressure in the dry region is a linear function of liquid saturation on a semi-log plot. Campbell and Shiozawa (1992) used this relationship and simply added a van Genuchten (1980) water content relationship to get the full capillary pressure curve where the parameters in the van Genuchten (1980) equation were refit to the data assuming zero liquid residual saturation. Subsequent models have all used the linear relationship observed by Campbell and Shiozawa (1992). The model proposed by Rossi and Nimmo (1994) is based on Brooks and Corey with zero residual saturation, which is equivalent to the expression of Campbell (1974), with the dry region function proposed by Campbell and Shiozawa (1992) in the low liquid saturation region. Two forms were presented by Rossi and Nimmo (1994) – a sum model and a junction model. The sum model adds the two components, while the junction model joins the two components imposing a continuous first derivative. Model parameters were determined by refitting the data. Fayer and Simmons (1995) replaced the residual saturation in the van Genuchten relationship with a form of the Campbell and Shiozawa (1992) function, and again refit the data. They also provided a preliminary methodology to estimate the refitting parameters from existing fits, which would make refitting unnecessary. Finally, Morel-Seytoux and Nimmo (1999) extended the Brooks and Corey model into the dry region using the Rossi and Nimmo (1994) junction model expression. The data did not have to be refit as existing parameters could be used in their model.

The data-model comparisons for all these approaches are generally good. Based on visual observation, the fit of Ross (1991) is reasonable, while the model of Campbell and Shiozawa (1992) shows considerable improvement. The models of Rossi and Nimmo (1994), Fayer and Simmons (1995), and Morel-Seytoux and Nimmo (1999) all give good data-model comparisons as exemplified by goodness of fit parameter values generally greater than 0.95 as reported by Morel-Seytoux and Nimmo (1999). As a practical matter, there is little to choose among the last three approaches other than the ease of implementation.

As noted above, most of the approaches necessitate refitting the appropriate equations to the data. If the original experimental data are available, this approach is the obvious choice. However, there are numerous existing fits to data, such as tabulated in Stephens (1996) and elsewhere, where the original data are not available. Therefore, it would be preferable to have a method that could use existing fits. The only methods that make use of existing fits are Fayer and Simmons (1995) and Morel-Seytoux and Nimmo (1999). The Fayer and Simmons (1995) approach uses existing fits to estimate the parameters in their modified capillary pressure expression. The generality of this estimation procedure is unknown. Morel-Seytoux and Nimmo (1999) merge existing capillary pressure curves with a dry region expression such that existing fits can be directly employed.

While using an existing capillary pressure curve fit is a practical advantage, it is not without its shortcomings. The existing fit is obviously dependent on the range of data used. Ideally, it should not include any of the data in the dry region, where the Campbell

and Shiozawa (1992) expression is more appropriate. If the original data are available, the selected equation set should be refit to these data. If the original data are not available, there is little choice but to use the existing fit and be aware of possible shortcomings.

The same issue of using an existing fit or refitting the data applies to relative permeability. Again, if the data are available, they curves should be refit to the data. However, in the case where an existing fit which is either extended or modified, the relative permeability fit may also be altered by this refitting procedure. Fayer and Simmons (1995) discuss the effect of a modified capillary pressure expression on the relative permeability and only saw a difference in the dry region where relative permeability values are very small. In general, however, it may be preferable for relative permeability to use the original relationship and fit parameters because relative permeability data may have been used in the existing fit. This area deserves further investigation.

The present method is only concerned with the capillary pressure curve; the relative permeability curve is not changed. The capillary pressure curve is extended to zero liquid saturation in a similar manner to the above studies, but it does not necessitate the refitting of experimental data. As discussed above, this feature is a significant advantage. The present approach is similar to the dry region modification of Morel-Seytoux and Nimmo (1999) in that it merges an existing capillary pressure curve with a dry region expression. However, the approach of Morel-Seytoux and Nimmo (1999) requires the

simultaneous solution of two nonlinear equations, while the present approach only requires a few iterations on a single equation as will be shown. Thus, the present approach is simple to implement in numerical simulations.

Model Development

As mentioned above, a problem exists with common two-phase capillary pressure functions as one approaches residual liquid saturation. It is important to recognize that the liquid residual saturation is only a fitting parameter and has no physical significance. The capillary pressure near residual liquid saturation approaches infinity, whereas it should approach a large but finite value at zero liquid saturation. This behavior is shown in Figure 1 for the van Genuchten function.

Existing capillary pressure curves such as van Genuchten need to be extended to oven dry, or zero liquid saturation, conditions. A reasonable description of oven dry conditions is a capillary pressure of 10^7 cm ($\sim 10^9$ Pa) at zero liquid saturation (Ross et al., 1991), although the capillary pressure may be higher for certain materials (Fayer and Simmons, 1995). Another capillary pressure value that is commonly employed is the wilting point usually taken to be 1.5×10^4 cm ($\sim 1.5 \times 10^6$ Pa). Direct suction measurements are often restricted to capillary pressures below the wilting point, and liquid flow is generally small at higher suctions. For capillary pressures greater than the wilting point, other measurement techniques are often used such as centrifuge, freezing point, or vapor pressure (Schofield, 1935; Nimmo, 1991).

For capillary pressures above the wilting point, water retention is generally governed by adsorption, which can be described by a logarithmic function as proposed by Campbell and Shiozawa (1992); this function is linear on a semi-log plot of $\log(P_{cap})$ vs. liquid saturation. This behavior will be clearly seen in the data presented later. A linear function on a semi-log plot can be expressed as

$$\log_{10}(P_{cap}) - \log_{10}(P_{cap}^*) = \gamma (S_t - S_t^*) \quad (1)$$

where

$$\gamma = - \frac{\log_{10} P_{cap}^0 - \log_{10} P_{cap}^*}{S_t^*} \quad (2)$$

P_{cap} is the capillary pressure, S_t is the liquid saturation, γ is the slope of the linear relationship, superscript 0 refers to the value at zero saturation (dry), and the superscript * is the value at the matching point which is discussed in the next section. This equation can be rearranged to reproduce the Campbell and Shiozawa (1992) expression if the pressure units are in m of head and the reference conditions (*) are taken to be 1 m of head. For the purposes of this model, this equation can be rewritten as

$$P_{cap} = 10^{(\gamma(S_t - S_t^*) + \log_{10} P_{cap}^*)} \quad (3)$$

The above equation fits the low moisture content capillary pressure data very well as will be obvious from the data-model comparison. One caution is that the amount of low moisture content capillary pressure data is very limited. Most of the data are for six different Washington State soils as measured by Campbell and Shiozawa (1992).

Another set of data is from Schofield (1935) which was used by Rossi and Nimmo (1994). For all these data, a linear equation on a semi-log plot gives a good representation of the low moisture content data.

Campbell et al. (1993) compared their simple linear relationship for the water sorption isotherm with the more complex model of Fink and Jackson (1973). The model of Campbell and Shiozawa (1992) only requires the determination of a single parameter, while the Fink and Jackson (1973) model uses three fitting parameters for the water sorption isotherm. Comparisons presented by Campbell et al. (1993) show that the simplified relationship given above fits the data about as well as the more complex model of Fink and Jackson (1973) for many soils. While there are some soils where the model of Fink and Jackson is superior, such as peat moss, the majority of the fits are similar.

Present Approach

The present approach is based on the van Genuchten function; other functions such as Brooks and Corey and Luckner et al. can easily be used if desired. In the present approach, the standard capillary pressure functional form is retained. At some point along the curve as one approaches residual liquid saturation, the capillary pressure function switches from the standard function to the logarithmic form given by equation (3) to describe the capillary pressure behavior at low liquid saturations. This point is determined by evaluating the point where a logarithmic extension based on the local slope would result in a capillary pressure of about 10^9 Pa ($\sim 10^7$ cm), or any other desired

value, at zero liquid saturation. This strategy allows for the use of existing numerical fits to capillary pressure data without the need of refitting the data.

This same general approach of using existing curve fits has also been used by Morel-Seytoux and Nimmo (1999). They merged the Rossi and Nimmo (1994) and Brooks and Corey expressions, requiring the simultaneous solution of two nonlinear equations. The present approach is simpler, and admittedly less elegant, in that it simply extends the van Genuchten capillary pressure curve to the desired dry value. By its simplicity, it only requires a few iterations on a single equation to produce the dry region capillary pressure curve.

The procedure described above is most easily visualized on a semi-log plot of $\log(P_{cap})$ vs. liquid saturation as depicted in Figure 1. On this plot, the extension of the curve according to the Campbell and Shiozawa (1992) expression is linear. Extensions to the van Genuchten capillary pressure curve are shown for various liquid saturation matching points (S_{ℓ}^*). As is clearly seen, the capillary pressure at zero liquid saturation increases dramatically as the liquid saturation matching point value decreases.

van Genuchten Development

The van Genuchten capillary pressure function written in terms of effective liquid saturation is

$$P_{cap} = \frac{1}{\alpha} (S_{\ell e}^{-1/n} - 1)^{1/n} \quad (4)$$

where

$$S_{te} = \frac{S_t - S_{tr}}{S_{ts} - S_{tr}} \quad (5)$$

α is a van Genuchten fitting parameter related to the air entry pressure, m and n are fitting parameters, S_{te} is the effective liquid saturation, and S_{tr} is the liquid residual saturation.

The slope of the van Genuchten function at any point on this semi-log scale is

$$\begin{aligned} \frac{d(\log_{10} P_{cap})}{dS_t} &= \log_{10} e \frac{1}{P_{cap}} \frac{dP_{cap}}{dS_t} \\ &= -\log_{10} e \frac{1}{S_t - S_{tr}} \frac{1}{nm} \frac{1}{1 - S_{te}^{1/n}} \end{aligned} \quad (6)$$

The intercept on the P_{cap} axis is simply

$$P_{cap}^0 = 10^{\left(\log_{10} P_{cap} - S_t \frac{d(\log_{10} P_{cap})}{dS_t} \right)} \quad (7)$$

or

$$P_{cap}^0 = 10^{\left(\log_{10} P_{cap} + \log_{10} e \frac{S_t}{S_t - S_{tr}} \frac{1}{nm} \frac{1}{1 - S_{te}^{1/n}} \right)} \quad (8)$$

where the slope is multiplied by the local liquid saturation to get the intercept at zero saturation. This modified capillary pressure curve consists of two regions. Region 1 is the adsorption region, which is described by a logarithmic function. Region 2 can be termed the capillary flow region, which is described by the standard van Genuchten

function (or any other desired function) where any previous fitting parameters are retained. The two regions meet where the extension of the existing capillary pressure curve results in the desired capillary pressure at zero saturation. Thus, the modified capillary pressure function has a continuous first derivative. The transition between these regions is at the matching point S_t^* , which is easily calculated by the equation

$$P_{cap}^0 = 10^{\left(\log_{10} P_{cap}^* + \log_{10} e \frac{S_t^*}{S_t^* - S_{tr}} \frac{1}{mm} \frac{1}{1 - S_{te}^{*/m}} \right)} \quad (9)$$

or

$$\log_{10} P_{cap}^0 = \log_{10} \left(\frac{1}{\alpha} \left(S_{te}^{*/m} - 1 \right)^{1/n} \right) + \log_{10} e \frac{S_t^*}{S_t^* - S_{tr}} \frac{1}{mm} \frac{1}{1 - S_{te}^{*/m}} \quad (10)$$

where

$$S_{te}^* = \frac{S_t^* - S_{tr}}{S_{ts} - S_{tr}} \quad (11)$$

and P_{cap}^0 is taken to be 10^7 cm (10^9 Pa) or any other oven dry value. The value of S_t^* is determined by iteration. For example, one can estimate S_t^* and calculate the value of P_{cap}^0 , which will be different from the desired value. Based on this result, the estimated value of S_t^* can be adjusted until the appropriate value of P_{cap}^0 is obtained. Determination of S_t^* generally only requires about 4-5 iterations.

Data-Model Comparison

The results of the present model are shown in this section for the six data sets from Campbell and Shiozawa (1992); these data were also used by Rossi and Nimmo (1994), Fayer and Simmons (1995), and Morel-Seytoux and Nimmo (1999). The data were converted from gravimetric water content (g/g) and potential (J/kg) to liquid saturation and capillary pressure (Pa) by assuming a soil bulk density of 1000 kg/m^3 , consistent with Fayer and Simmons (1992), and a water density of 1000 kg/m^3 . The fitting parameters to the van Genuchten functions as presented by Fayer and Simmons (1995) are used in this comparison which are based on the Mualem-based formulation of the van Genuchten function such that $m=1-1/n$.

These fitting parameters, which are summarized in Table 1, are only for the data with capillary pressure less than or equal to the wilting point, or $1.5 \times 10^4 \text{ cm}$ ($\sim 1.5 \times 10^6 \text{ Pa}$). The porosity, ϕ , is assumed equal to the saturated volumetric moisture content. Two data points for the Salkum soil are at moisture contents ($\theta = 0.481, 0.485$) greater than the saturation moisture content ($\theta_{1s} = 0.479$) and are therefore not shown in the data-model comparison. The values of S_e^* obtained from iterative solution of equation (10) for a P_{cap}^0 of 10^9 Pa are also shown. In this data-model comparison, S_{eS} is assumed equal to 1.0.

The extrapolation of the limited data fit is similar to what might occur if one was to obtain van Genuchten fitting parameters from an existing tabulation such as in Stephens (1996). In that case, the fitting parameters are available but the actual data are not, so

refitting the curve would not be possible. In that case, the logarithmic extension would be made without the benefit of the data.

As seen in Figure 2, the present approach results in good agreement between the van Genuchten curve with the logarithmic extension and the experimental data. The data-model comparison for the Salkum soil is not as good as the other soils but it still reasonable. For all six soils, the fits with the present approach are similar to the fits presented by Rossi and Nimmo (1994), Fayer and Simmons (1995), and Morel-Seytoux and Nimmo (1999). The R^2 values for the dry region extension range from 0.935 to 0.987 and are given in Table 1. While the fits are similar, the present approach has the distinct advantage of using existing data fits for the capillary pressure curve as well as a simple procedure for determining the matching point, S_e^* .

Also shown in Table 1 are the values of the matching location in terms of saturation, S_e^* , and capillary pressure, P_{cap}^* . These parameters are simply fitting parameters and have limited physical significance. The values of P_{cap}^* are of some interest because Campbell and Shiozawa (1992) suggested that the linearity of the dry region extends down to about 10 m suction, or 100 kPa. Note that all the values listed in Table 1 are greater than this suggested lower limit, so the dry region extension should be applicable.

Conclusions

A simple extension of capillary pressure functions to zero liquid saturation is proposed. Sample results have been generated for the van Genuchten capillary pressure

function, which shows very good agreement with the data over the entire range of liquid saturations down to oven dryness. The advantage of the present approach is that the capillary pressure expression does not need to be refit to the data; instead, existing fits can be used. Refitting the data can be difficult or impossible if the original data are not available. The present approach is a simple and easy extension of the capillary pressure curves that retains the original fit at higher saturations and improves the fit at lower saturations.

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Nomenclature

m, n	van Genuchten fitting parameters
P_{cap}	capillary pressure
P_{cap}^0	capillary pressure at zero saturation
P_{cap}^*	capillary pressure at S_r^*
S_r	liquid saturation
S_r^*	liquid saturation matching point

Greek

α	van Genuchten fitting parameter
γ	slope of the capillary pressure curve in the linear region
ϕ	porosity

Subscripts

e	effective
ℓ	liquid
r	residual
s	saturated

Superscript

0	value at zero saturation or moisture content
*	value at matching point

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Table 1
Soil Fitting Parameters¹

Soil	ϕ	S_{lr}	$1/\alpha$ (Pa)	n	$m (=1-1/n)$	S_l^*	P_{cap}^* (kPa)	R^2
Palouse	0.442	0.158	9520.	1.49	0.329	0.231	1454.	0.987
Palouse B	0.549	0.	3740.	1.19	0.160	0.251	5371.	0.982
Walla Walla	0.398	0.171	9810.	1.64	0.390	0.219	848.	0.977
Salkum	0.479	0.	21800.	1.35	0.259	0.0647	56032.	0.935
Royal	0.352	0.188	12600.	2.48	0.597	0.203	182.	0.981
L soil	0.203	0.167	3190.	2.09	0.522	0.186	106.	0.982

¹van Genuchten Parameters are from Fayer and Simmons, 1995.

Figure 1

Representative van Genuchten Capillary Pressure Function Including Linear Extension

Figure 2

Data-Model Comparison for the Present Extension to the van Genuchten Capillary Pressure Curve

(a) Palouse

(b) Palouse B

(c) Walla Walla

(d) Salkum

(e) Royal

(f) L soil

Palouse

Palouse B

Walla Walla

Salkum

Royal

L-Soil