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Modeling of soil water retention from saturation to oven dryness

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Abstract. Most analytical formulas used to model moisture retention in unsaturated porous media have been developed for the wet range and are unsuitable for applications in which low water contents are important. We have developed two models that fit the entire range from saturation to oven dryness in a practical and physically realistic way with smooth, continuous functions that have few parameters. Both models incorporate a power law and a logarithmic dependence of water content on suction, differing in how these two components are combined. In one model, functions are added together (model "sum"); in the other they are joined smoothly together at a discrete point (model "junction"). Both models also incorporate recent developments that assure a continuous derivative and force the function to reach zero water content at a finite value of suction that corresponds to oven dryness. The models have been tested with seven sets of water retention data that each cover nearly the entire range. The three-parameter sum model fits all data well and is useful for extrapolation into the dry range when data for it are unavailable. The two-parameter junction model fits most data sets almost as well as the sum model and has the advantage of being analytically integrable for convenient use with capillary-bundle models to obtain the unsaturated hydraulic conductivity.

Introduction

In numerical modeling of water flow and solute transport in unsaturated porous media a simple analytical function is desirable and often necessary for representing the water retention curve, the relation between water content and matric suction. Usually, a mathematical function is chosen and its parameter values are determined by a regression analysis on the available data [*Bruce and Luxmoore*, 1986].

Various functions that describe the water retention curve are in use [e.g., *Brooks and Corey*, 1966; *van Genuchten*, 1980]. Generally, they are successful at high and medium water contents but often give poor results at low water contents [*Nimmo*, 1991; *Ross et al.*, 1991]. This may pose little difficulty for some applications, such as wetlands studies or humid region agriculture, but others, including water flow and contaminant transport in arid regions, require a more accurate representation of the hydraulic characteristics over the whole range of saturation. For fine-textured media the high-suction range can be important even with water content remaining high.

A further motivation for creating a whole range model of water retention is that there are few sets of measured data containing observations in the range of suction greater than 1.5×10^4 cm water, the value often assumed as the maximum for water extraction by plants. Because measurements at this value can be difficult and time consuming in order to ensure equilibrium, many data sets end at suctions even closer to zero. Thus it would be of great value to have a model that can reliably extrapolate the water retention curve beyond the driest measured point.

Another issue related to traditional water retention models is that they either do not allow water content to be zero, an assumption that is physically unrealistic [*Nimmo*, 1991], or they allow it to be zero only at infinite suction. In practice, zero water content is defined as oven dryness, which corresponds to a finite suction. *Ross et al.* [1991] proposed a correction of the Brooks-Corey model that makes water content $\theta = 0$ at a finite value of suction Ψ_d approximating oven dryness. The value of Ψ_d depends on the temperature, pressure, and humidity in which the soil is dried; unfortunately, the procedure is imperfectly standardized and can be subject to different conditions in different laboratories [*Gardner*, 1986]. For the typical case of oven drying at 105°–110°C in a room at 50% relative humidity, however, the value of $\Psi_d = 10^7$ cm water proposed by *Ross et al.* [1991] is reasonably accurate. The *Ross et al.* [1991] correction improves the modeling of soil water retentivity in the low water content range, but it leaves room for further improvements in terms of goodness of fit and physical interpretation, especially regarding modeling over the whole range of saturation.

A modification of the van Genuchten model has been proposed by *Campbell and Shiozawa* [1992] for improving fits to dry range data. Their equation fits the data very well in the range considered, but it has four parameters, one more than the most commonly used form of the van Genuchten equation. Other disadvantages are that the water content

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theoretically goes to zero only at infinity and that it tends to an infinite value when the suction approaches zero.

In the present study we investigate possible improvements in modeling soil water retentivity with the goal of developing practical models, still physically realistic, that can represent with the minimum possible number of parameters the retention curve over the entire range of saturation. This investigation has led to two models based on the same assumptions but differing in mathematical details.

Theory

For physical realism and to prevent problems in numerical calculations, a water retention model must be analytically represented by a continuous function with at least a continuous first derivative. In this paper, functions with these characteristics will be designated as smooth.

In general, a second-order continuous function would be desirable in order to guarantee the specific water capacity function, defined as $d\theta/d\Psi$, to be a smooth function also. In this study, however, we address the less strict requirements that the retention curve be smooth and the specific water capacity be continuous.

General Features

Both models proposed here are based on a modified form of the *Brooks and Corey* [1966] model with residual saturation taken as zero, which is also equivalent to the equation used by *Campbell* [1974]. This formula is a power law for matric suction Ψ greater than the air entry value Ψ_o and can be written

$$\frac{\theta}{\theta_s} = 1 \qquad 0 \le \Psi \le \Psi_o$$
$$\frac{\theta}{\theta_s} = \left(\frac{\Psi_o}{\Psi}\right)^{\lambda} \qquad \Psi \ge \Psi_o \tag{1}$$

where θ is the volumetric water content, and θ_s is the saturated water content or the maximum value of θ if air trapping is considered. The parameters Ψ_o, and λ, and sometimes θ_s are usually fitted to measured data for each soil.

We chose the power law function as a starting basis because of its simplicity and its demonstrated ability to well represent the retention curve in the middle range of saturation [*Brooks and Corey*, 1966]. Another advantage is that it can be physically interpreted in terms of self-similar scaling of soil pore sizes, as *Tyler and Wheatcraft* [1990] have shown.

One of the shortcomings of the Brooks-Corey model is that it presents a sharp discontinuity in the derivative at Ψ_o. As a first modification of (1), we have adopted the parabolic correction near saturation proposed by *Hutson and Cass* [1987], which replaces the sharp corner with a smooth curve. The result is a smoothly joined two-part retentivity equation with no more parameters than the original equation.

The Brooks-Corey model, however, does not adequately represent the data at very high suctions; the simple power law consistently overestimates the water content in this range [*Campbell and Shiozawa*, 1992]. This may be a matter of the Brooks-Corey model representing capillarity better than adsorption.

As a second modification to (1), we have adopted the correction for the dry end of the curve proposed by *Ross et al.* [1991] that makes water content $\theta = 0$ at a finite value of suction Ψ_d. Given a water retention equation $\theta = f(\Psi)$, such a correction consists simply of modifying it to $\theta = f(\Psi) - f(\Psi_d)$, again not adding any extra parameters to the original model if Ψ_d is known.

The main modification of the Brooks-Corey equation that we propose is based on the assumption that in the dry range of the water retention curve the water content becomes approximately proportional to the logarithm of suction. This assumption is consistent with the *Bradley* [1936] adsorption theory which considers adsorbed molecules to build up in a layered film, in which the net force of electrical attraction diminishes with each additional layer. *Orchiston* [1953] also tested the proportionality of θ to the logarithm of suction and found that it gave good fits to low-θ measurements. There are then two different behaviors to be represented in our soil water retention models: a power law behavior at high and medium water content where the capillary retention mechanism is dominant and a logarithmic behavior at low water contents where adsorption is dominant.

The two models we propose here differ in how these two components are combined: The sum model considers the two functions added, whereas the junction model considers the two components jointed together. The two models are characterized by a different mathematical formulation and a different number of fitting parameters that result in some differences in the goodness of fit and differences in applicability for various purposes.

It should be noted that every analytic model has several parameters, some of which can be directly determined from measurements while the others have to be fitted to a whole data set. Some parameters may be directly determined in some cases and fitted in others. In this paper we designate the number of parameters of a model as the number of fitted parameters. For consistency the fitted parameters here are counted as those that would always be fitted; in particular, θ_s and Ψ_d are not considered as fitted parameters but as known values. Furthermore, on account of the different role played by the parameters in the different formulations, the parameter values obtained through the regression analyses are not expected to be the same, neither for the sum and junction models nor for the Brooks-Corey model from which they are derived.

Formulation of Three-Parameter Sum Model

The first model combines the power function with the logarithmic function by adding them as follows

$$\frac{\theta}{\theta_s} = \theta_I = 1 - c\left(\frac{\Psi}{\Psi_o}\right)^2 \qquad 0 \le \Psi \le \Psi_i$$
$$\frac{\theta}{\theta_s} = \theta_{II} = \left[\left(\frac{\Psi_o}{\Psi}\right)^{\lambda} - \left(\frac{\Psi_o}{\Psi_d}\right)^{\lambda}\right] + \alpha \ln\left(\frac{\Psi_d}{\Psi}\right) \qquad \Psi_i \le \Psi \le \Psi_d \tag{2}$$

The term θ_I represents the *Hutson and Cass* [1987] parabolic curve that joins to the Brooks-Corey function at the junction point Ψ_i. The *Ross et al.* [1991] correction can be recognized in the expression for θ_{II}.

If θ_s and Ψ_d are known, the number of unknown parameters in (2) is five (c, Ψ_i, Ψ_o, λ, α), but two of these are determined by the conditions that ensure the continuity of

both the function and its first derivative at Ψ_i, leaving just three free parameters. Such continuity conditions are expressed by the system of two equations

$$\theta_I(\Psi_i) = \theta_{II}(\Psi_i)$$
$$\frac{\partial \theta_I}{\partial \Psi}(\Psi_i) = \frac{\partial \theta_{II}}{\partial \Psi}(\Psi_i) \tag{3}$$

Considering two of the unknown parameters as dependent variables and the remaining three as independent variables, (3) allows us to express any two chosen parameters as functions of the others. Substituting these expressions for the two dependent parameters into (2) leaves three parameters, whose values are then optimized through a regression analysis on the available data. In our test of the model the two parameters c and α are explicitly determined as analytical functions of Ψ_o, λ, and Ψ_i. These three remain then the only free parameters to be fitted. An advantage of this formulation is that the relationships among the parameters can be solved analytically with respect to the dependent ones.

The sum model, defined in (2), globally represents then a continuous analytical function with continuous first derivative that can be easily inserted in a numerical scheme with three fitting parameters, as many as the usual version of the *van Genuchten* [1980] model.

Formulation of Two-Parameter Junction Model

The second model combines the power law and the logarithmic function with a junction rather than a summation

$$\frac{\theta}{\theta_s} = \theta_I = 1 - c\left(\frac{\Psi}{\Psi_o}\right)^2 \qquad 0 \le \Psi \le \Psi_i$$
$$\frac{\theta}{\theta_s} = \theta_{II} = \left(\frac{\Psi_o}{\Psi}\right)^{\lambda} \qquad \Psi_i \le \Psi \le \Psi_j \tag{4}$$
$$\frac{\theta}{\theta_s} = \theta_{III} = \alpha \ln\left(\frac{\Psi_d}{\Psi}\right) \qquad \Psi_j \le \Psi \le \Psi_d$$

In this case there are six parameters and four conditions to be satisfied in order to impose the continuity of the global function and its first derivative at the two junction points. The four parameters c, Ψ_i, Ψ_j, and α are determined as analytical functions of the remaining two through the equations

$$\theta_I(\Psi_i) = \theta_{II}(\Psi_i) \qquad \frac{\partial \theta_I}{\partial \Psi}(\Psi_i) = \frac{\partial \theta_{II}}{\partial \Psi}(\Psi_i)$$
$$\theta_{II}(\Psi_j) = \theta_{III}(\Psi_j) \qquad \frac{\partial \theta_{II}}{\partial \Psi}(\Psi_j) = \frac{\partial \theta_{III}}{\partial \Psi}(\Psi_j) \tag{5}$$

Applying a procedure analogous to the one described for the sum model, the junction model may be characterized by two independent parameters, Ψ_o and λ. This is as many as the original Brooks-Corey model and one fewer than the sum model.

A cubic polynomial could be employed for the wet range instead of the parabolic correction proposed by *Hutson and Cass* [1987]. That could have a possible advantage in guaranteeing second-order continuity of the whole function and especially a zero second derivative at saturation. This function is not used in either the sum or the junction model, however, because an attempt to incorporate it in order to have a continuous second derivative for the whole range without adding extra parameters did not lead to an analytical determination of the dependent parameters.

Table 1. Summary of Soil Textural Classes

Soil	Textural Class	Measured Properties		
		Sand	Clay	Silt
Palouse[a]	Silt loam	0.113	0.205	0.682
Palouse B[a]	Silty clay	0.093	0.468	0.439
Walla Walla[a]	Silt loam	0.228	0.139	0.633
Salkum[a]	Silt loam	0.190	0.225	0.585
Royal[a]	Sandy loam	0.536	0.145	0.319
L-soil[a]	Sand	0.888	0.051	0.061
Rothamsted[b]	Loam	Not available		

[a]From *Campbell and Shiozawa* [1992].
[b]From *Schofield* [1935].

The junction model has the advantage that it is integrable in closed form for use in a conductivity model such as that of *Mualem* [1976]. According to this model, the relative hydraulic conductivity, the ratio between the unsaturated and saturated hydraulic conductivity, can be expressed as

$$K_r(\theta) = \sqrt{\frac{\theta}{\theta_s}}\,\frac{I^2(\theta)}{I^2(\theta_s)} \tag{6}$$

where

$$I(\theta) = I_{III}(\theta) \qquad 0 \le \theta \le \theta_j$$
$$I(\theta) = I_{II}(\theta) \qquad \theta_j \le \theta \le \theta_i \tag{7}$$
$$I(\theta) = I_I(\theta) \qquad \theta_i \le \theta \le \theta_s$$

and

$$I_{III}(\theta) = \frac{\alpha}{\Psi_d}\left[\exp\left(\frac{1}{\alpha}\frac{\theta}{\theta_s}\right) - 1\right]$$
$$I_{II}(\theta) = I_{III}(\theta_j) + \frac{1}{\Psi_o}\frac{\lambda}{\lambda+1}\left[\left(\frac{\theta}{\theta_s}\right)^{(\lambda+1)/\lambda} - \left(\frac{\theta_j}{\theta_s}\right)^{(\lambda+1)/\lambda}\right] \tag{8}$$
$$I_I(\theta) = I_{II}(\theta_i) + \frac{2c^{1/2}}{\Psi_o}\left[\left(1 - \frac{\theta_i}{\theta_s}\right)^{1/2} - \left(1 - \frac{\theta}{\theta_s}\right)^{1/2}\right]$$
$$\theta_i = \theta(\Psi_i) \qquad \theta_j = \theta(\Psi_j)$$

Without tests against reliable data the accuracy of the prediction of unsaturated hydraulic conductivity through (7) and (8) is not known.

Results and Discussion

Both models presented above were tested with data from seven soils of a wide range of texture [*Campbell and Shiozawa*, 1992; *Shiozawa and Campbell*, 1991; *Schofield*, 1935], as listed in Table 1. These data sets have been chosen

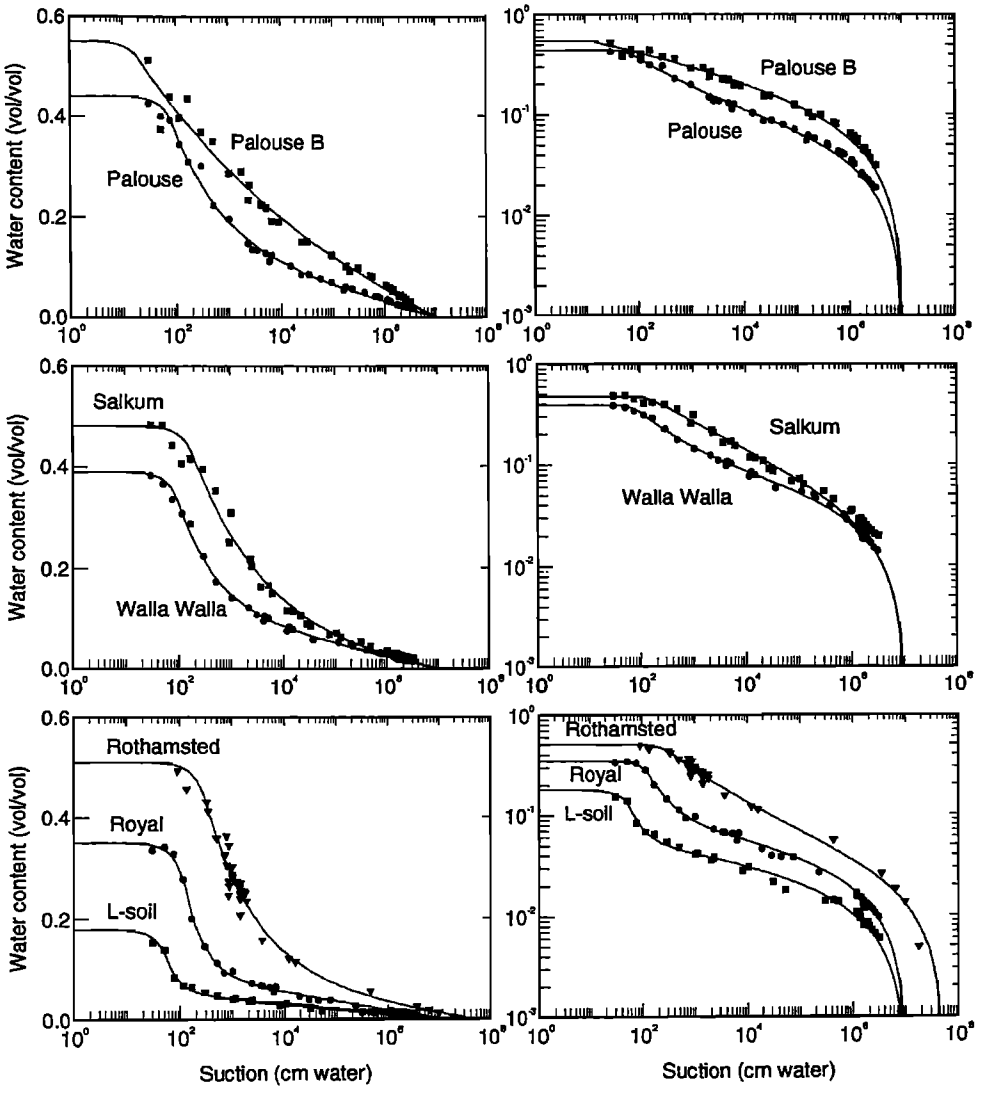

Figure 1. Model sum fitted to six data sets from *Campbell and Shiozawa* [1992] and one data set (Rothamsted) from *Schofield* [1935]. Curves and data are plotted on both semilog and log-log scales.

because they cover a large range, almost six orders of magnitude in suction, from nearly saturated to nearly oven dry. For each data set, both models have been fitted to the data using the Standards Time Series and Regression Package nonlinear least squares analysis [*Donaldson and Tryon*, 1983]. The parameters whose values are determined through the regression analyses are Ψ_o, λ, and Ψ_i for the sum models and Ψ_o and λ for the junction model.

We did not treat θ_s and Ψ_d as free parameters but rather assigned them values based on inspection of the data. In many cases, θ_s will be known or well approximated by measurements, and Ψ_d can be computed if the conditions of oven drying are known. Regarding Ψ_d, for the chosen data sets, since each includes measurements that closely approach zero water content, a short linear extrapolation on a semilog plot provided a suitable value of 10^7 cm water for the six soils from *Campbell and Shiozawa* [1992] and a value of 5×10^7 cm water for the *Schofield* [1935] data. This difference probably results from different conditions of water content measurements. As a test, we did some analyses with Ψ_d as a free parameter, finding that the values of the other fitted parameters had a negligible difference from the case with Ψ_d fixed, and the optimized values of Ψ_d were very close to the chosen ones.

Figure 1 shows results of fitting the three-parameter sum model to the seven chosen data sets, while Figure 2 shows results obtained using the two-parameter junction model. The figures include the results plotted in both semilog and log-log forms, since the different scales highlight different characteristics of the data and the fitted functions.

Tables 2 and 3 present the values of the parameters determined by the regression analysis as well as the resulting residual standard deviations σ. The residual standard deviation is calculated as the square root of the residual sum of squares divided by the number of degrees of freedom [*Draper and Smith*, 1981].

As the graphs and tables show, the fitting is generally very good for both models. In particular, the sum model fits all data sets well. The junction model fits well the Palouse, Palouse B, Walla Walla, Salkum, and Rothamsted data. For

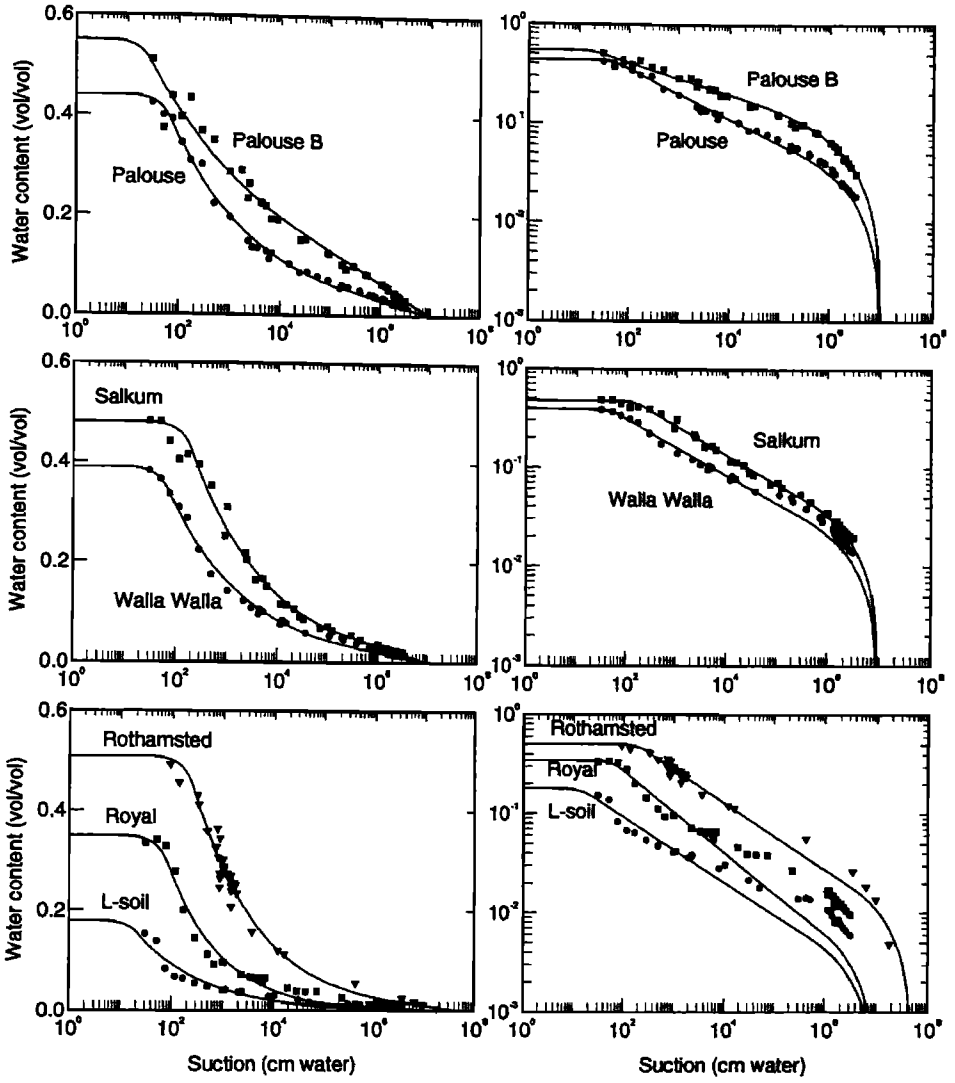

Figure 2. Model junction fitted to six data sets from *Campbell and Shiozawa* [1992] and one data set (Rothamsted) from *Schofield* [1935]. Curves and data are plotted on both semilog and log-log scales.

Table 2. Summary of Soil Parameters and Standard Deviations From the Fitting of Model Sum to the Seven Data Sets

Soil	θ_s, vol/vol	Ψ_o, cm water	λ	Ψ_j, cm water	σ, vol/vol
Palouse[a]	0.44	22.8	0.47	89.3	0.0088
Palouse B[a]	0.55	1.1	0.15	19.6	0.0201
Walla Walla[a]	0.39	35.6	0.61	104.6	0.0062
Salkum[a]	0.48	83.6	0.29	185.7	0.0166
Royal[a]	0.35	72.7	1.24	137.2	0.0045
L-soil[a]	0.18	32.7	1.83	57.1	0.0034
Rothamsted[b]	0.51	128.2	0.43	304.9	0.0229

The parameters θ_s and ψ_d were fixed in accordance with measured data.
[a] $\Psi_d = 1 \times 10^7$ cm water.
[b] $\Psi_d = 5 \times 10^7$ cm water.

the other two soils, although the values of the standard deviation are still low, the junction model works less well in the low water content range, evident mainly on the log-log plots. It is expected that in some degree the junction model will provide fits inferior to those of the sum model, since it is characterized by one fewer parameter.

The high quality of the fits at low theta supports the importance of the logarithmic component. The log-log plots in Figures 1 and 2 show how the observed data deviate from the simple power law formula, dropping faster to zero water content, whereas both the sum and junction models follow the real data behavior. This result is clear also from Figure 3 which shows the sum, junction, and Brooks-Corey models fitted to one of the soils.

For the junction model the deviation from the power law begins exactly at the second junction point Ψ_j, where the function becomes completely logarithmic. This point is analytically determined from (5) as $\Psi_d \exp(-1/\lambda)$. The

Table 3. Summary of Soil Parameters and Standard Deviations From the Fitting of Model Junction to the Seven Data Sets

Soil	θ_s, vol/vol	Ψ_o, cm water	λ	Ψ_j, cm water	σ, vol/vol
Palouse[a]	0.44	43.4	0.25	1.9×10^5	0.0089
Palouse B[a]	0.55	16.7	0.16	2.0×10^4	0.0210
Walla Walla[a]	0.39	44.6	0.28	2.9×10^5	0.0086
Salkum[a]	0.48	131.2	0.29	3.3×10^5	0.0159
Royal[a]	0.35	53.8	0.41	8.8×10^5	0.0154
L-soil[a]	0.18	13.3	0.33	4.7×10^5	0.0098
Rothamsted[b]	0.51	176.3	0.34	2.6×10^6	0.0227

The parameters θ_s and ψ_d were fixed in accordance with measured data. Ψ_j has been calculated from the fitted parameters Ψ_o and λ.

[a] $\Psi_d = 1 \times 10^7$ cm water.

[b] $\Psi_d = 5 \times 10^7$ cm water.

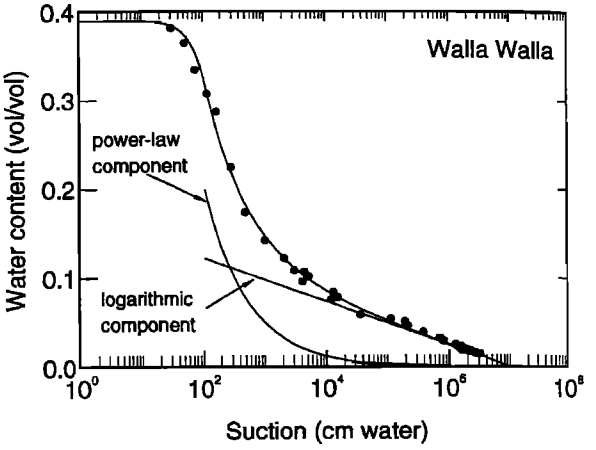

Figure 4. Model sum fitted to data of Walla Walla soil. The power law and logarithmic components, both including the *Ross et al.* [1991] correction, are plotted separately.

calculated values of Ψ_j for all the soils examined are given in Table 3.

Because the sum model does not have a distinct transition from the power law to the logarithmic function it is not possible to determine analytically a single point at which deviation begins. The two functions added behave as expected, however, with each of the two behaviors dominating a different range of suction. The results in the example of Figure 4, qualitatively similar to the ones for the other soils, show that at lower suctions the power law component has a greater influence but at higher suctions the logarithm, going to zero more slowly, takes over.

In order to assess the ability of the model to extrapolate observed data in the dry range, regression analyses have been performed on subsets of data that exclude all measured points with suction greater than a certain cutoff value Ψ_c. Where the value of Ψ_d is known, this procedure is in effect less an extrapolation than an interpolation between the measurements and Ψ_d, but we refer to it as extrapolation since the modeling is out of the range of measured data. We did these calculations for both models with all seven soils over the possible Ψ_c values from the maximum measured Ψ to the minimum for which there were adequate data for the computations. In each case the resulting curves provided good fits to the whole data set for Ψ_c values as low as a few thousands, or sometimes hundreds, of centimeters water. In most cases, model sum produced better extrapolated fits, though with the lower Ψ_c values, and model junction gave better fits for Palouse B, Walla Walla, and Rothamsted.

Tables 4 and 5 present the residual standard deviations computed respectively from the fitting of models sum and junction to the whole data sets and to data subsets obtained with two cutoff values of different order of magnitude. Note that while the regressions are based on the subsets, the standard deviations are computed based on all the data.

As an example, Figure 5 illustrates two of these fits for model sum and a cutoff value of 1.5×10^4 cm water. The results are for two soils: the Royal that showed one of the best agreements and the Palouse soil that was the worst. Only the results for Rothamsted resembled those for Palouse, while results for other soil types resembled those for Royal.

The question of the minimum number of data points or minimum Ψ_c value required for a given medium is difficult to answer here because the seven data sets show considerable scatter and are fairly sparse in the wet part of the range.

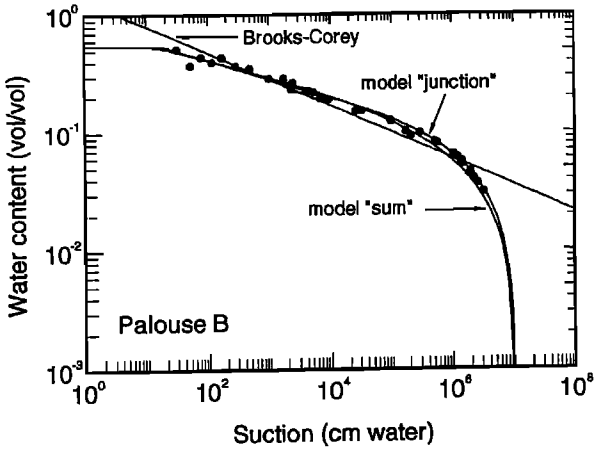

Figure 3. Comparison of Brooks-Corey, sum, and junction models fitted to Palouse B data.

Table 4. Summary of Residual Standard Deviations From the Fitting of Model Sum to Data Subsets Containing Only Data With Suction Less Than Different Cutoff Values

Soil	Cutoff value Ψ_c, cm water		
	1×10^8	1.5×10^4	5×10^3
Palouse	0.0088	0.0140	0.0259
Palouse B	0.0201	0.0208	0.0206
Walla Walla	0.0062	0.0069	0.0079
Salkum	0.0166	0.0170	0.0174
Royal	0.0045	0.0048	0.0050
L-soil	0.0034	0.0034	0.0036
Rothamsted	0.0229	0.0242	0.0333

The standard deviations are based on the whole data sets.

Table 5. Summary of Residual Standard Deviations From the Fitting of Model Junction to Data Subsets Containing Only Data With Suction Less Than Different Cutoff Values

Soil	Cutoff value Ψ_c, cm water		
	1×10^8	1.5×10^4	5×10^3
Palouse	0.0089	0.0102	0.0109
Palouse B	0.0210	0.0215	0.0225
Walla Walla	0.0086	0.0095	0.0105
Salkum	0.0159	0.0160	0.0181
Royal	0.0154	0.0162	0.0171
L-soil	0.0098	0.0101	0.0106
Rothamsted	0.0227	0.0227	0.0229

The standard deviations are based on the whole data sets.

Palouse B, for example, was successfully extrapolated with model junction and a Ψ_c of 1000 cm water, but this was done with only eight data points that appear to have a substantial random component from measurement uncertainty. With a greater quantity or quality of wet range data, lower values of Ψ_c may be acceptable.

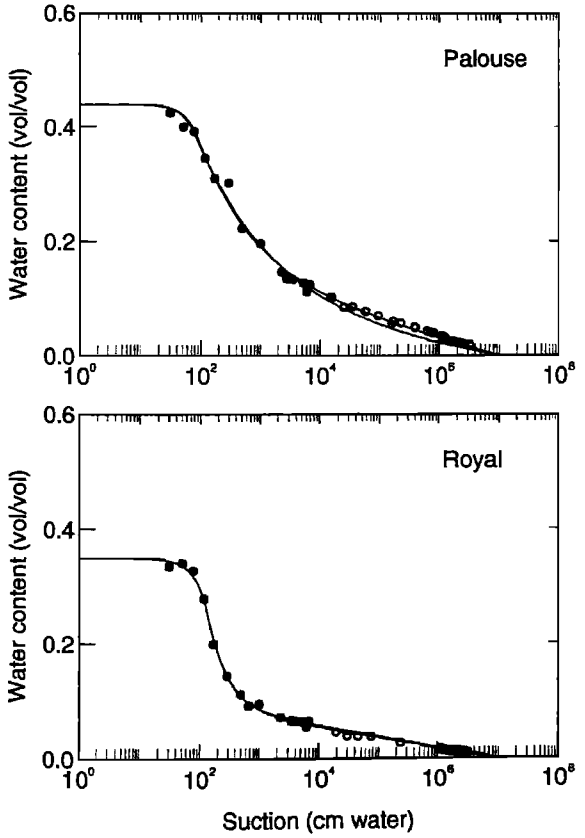

Figure 5. Comparison, for Palouse and Royal soils, between the curves fitted with model sum using the complete data sets and using subsets that include only data with suction less than 1.5×10^4 cm water.

Conclusions

We have proposed two models that realistically represent the soil water retention curve over the whole range of saturation with no more than three parameters. Both models are based on a power law function supplemented with a logarithmic function relating water content to suction in the high suction range. One model combines the power law with the logarithmic formula using a summation, whereas the other combines them using a junction. They both are continuous functions with continuous derivatives and have simple mathematical formulations.

The sum model, using three parameters, provides good fits over the whole range of saturation for all soil types considered. The reliability of this model, particularly in the high suction range, is also reflected in the high-quality extrapolation that it gives when fitted to limited data subsets. The results also confirm the appropriateness of the use of a finite value of suction for zero water content.

The junction model gives good fits for most media analyzed. With two parameters, as many as the original Brooks-Corey model assuming θ_s to be known, it improves the soil water retention modeling at low water contents. One of the junction model's advantages is that it is analytically integrable for easy use in a conductivity model such as *Mualem*'s [1976].

The goodness of fit of both models to measured data supports the validity of the assumption of proportionality between soil water content and logarithm of suction in the low water content range. The combination of this logarithmic dependence with other formulations developed for the high water content range produces a model that is practical and realistic from saturation to oven dryness.

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