RETC: A COMPUTER PROGRAM FOR ANALYZING SOIL WATER RETENTION AND HYDRAULIC CONDUCTIVITY DATA

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Detailed knowledge of the soil hydraulic properties (the soil water retention and hydraulic conductivity curves) is indispensable for predicting or managing the migration of water and dissolved constituents in unsaturated soils. Unfortunately, the hydraulic properties are difficult and cumbersome to determine experimentally, especially the hydraulic conductivity, ***K*, *as*** a function of water content, θ, or soil water pressure head, h. As an alternative to direct measurement of ***K(h),*** statistical pore-size distribution models have been developed to indirectly estimate the hydraulic conductivity from the more easily measured soil water retention curve, B(h). The most popular models of this type are the Burdine and Mualem models. Combination of these predictive models with the soil water retention functions of Brooks-Corey or van Genuchten yields relatively simple mathematical expressions for the unsaturated hydraulic conductivity curve.

This paper describes an optimization software package, RETC, useful for optimizing selected parameters in several analytical expressions for the unsaturated hydraulic properties. A previous version of the program has been widely used in research for predicting the hydraulic conductivity function using parameters fitted to observed water retention data. A new feature of RETC is that it is now possible to simultaneously optimize some or all potentially unknown parameters in the adopted models, leading to a maximum of five or six independent parameters in the Brooks-Corey models, and six or seven parameters in the Mualem-van Genuchten and Burdine-van Genuchten models. The exact number of unknowns depends on the assumed complexity of the soil water retention function. Selected examples are presented to illustrate the utility of RETC for calculating the hydraulic properties from known model parameters, for predicting the relative unsaturated hydraulic conductivity function from measured soil water retention data only, and for simultaneously optimizing measured soil water retention and hydraulic conductivity data.

INTRODUCTION

Two common expressions used for modeling one-dimensional soil water flow are

$$\frac{\partial\theta}{\partial t} = \frac{a}{\partial z}\left[D\frac{\partial\theta}{\partial z} - K\right] \tag{1}$$

$$C\frac{\partial h}{\partial t} = \frac{\partial}{\partial z}\left[K\frac{\partial h}{\partial z} - K\right] \tag{2}$$

where θ is the volumetric water content $[L^3L^{-3}]$, t is time [T], z is the vertical space coordinate or the distance from the soil surface [L], D is the soil water diffusivity $[L^2T^{-1}]$, ***K* is** the hydraulic conductivity $[LT^{-1}]$, C is the soil water capacity $[L^{-1}]$, and ***h* is** the soil

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water pressure head [L]. Note that $C=d\theta/dh$ and $D=K/C$. In this paper we use positive values for h in unsaturated soil (i.e., h denotes suction).

Modeling flow and transport in the vadose zone requires knowledge of the unsaturated hydraulic properties, i.e., the water retention function, $\theta(h)$, and the hydraulic conductivity function, $K(\theta)$ or $K(h)$, or the diffusivity function, $D(\theta)$. Various pore-size distribution models have been developed based on physico-empirical grounds [Brutsaert, 1967; Mualem, 1986]. These models depend on the pore- or particle-size distribution, which is usually derived from retention data using Laplace's equation for surface tension. Hence, soil water retention data need to be described with an analytical function before closed-form equations for the conductivity can be obtained. Analytical expressions for $\theta(h)$ are also attractive for mathematical modeling of flow and transport and for comparative analyses of the hydraulic properties of different soils. Popular models for $\theta(h)$ were presented by Brooks and Corey [1964] and van *Genuchten* [19801.

In this paper we will mainly deal with the description of the software package, RETC (RETention Curve), useful for optimizing the unknown parameters in several analytical expressions for the unsaturated soil hydraulic properties. The most important program features of RETC are reviewed, and examples are presented to illustrate the utility of RETC for estimating the hydraulic parameters from retention data only, or simultaneously from observed retention and hydraulic conductivity data. A more detailed description of the program is given in the report by van *Genuchten et al.* [1991].

MODEL FORMULATION

Retention Models

Two widely used expressions for describing the soil water retention function are

$$\theta = \begin{cases} \theta_s & \alpha h < 1 \\ \theta_r + \dfrac{\theta_s - \theta_r}{(\alpha h)^\lambda} & \alpha h \geq 1 \end{cases} \qquad \text{Brooks-Corey (BC)} \tag{3}$$

$$\theta = \theta_r + \frac{\theta_s - \theta_r}{[1 + (\alpha h)^n]^m} \qquad \text{van Genuchten (VG)} \tag{4}$$

where the subscripts r and s denote residual and saturated water contents, respectively, α is an empirical parameter whose inverse is frequently referred to as the air entry value [cf. Brooks and Corey, 1964], n and m are dimensionless empirical shape factors, and λ is a pore-size distribution index. For practical purposes, and because of the similarity of both models, this distribution index is also denoted as n in the program RETC.

Figures 1 and 2 show the reduced water content, $S_e=(\theta-\theta_r)/(\theta_s-\theta_r)$, versus the reduced pressure head according to (4). Various values for n were used in Figure 1 with two representative values form, viz. 0.1 (a) and 1 (b). The steepness of the curve increases with the value for n, whereas m determines the value for S_e when $h=1/\alpha$. In Figure 2 the product mn was kept constant at a representative value of 0.4. At low saturation values a unique limiting curve occurs for all values of n; at higher saturation values the limiting curve is reached for $n\to\infty$. The limiting curve can be obtained from the Brooks-Corey function, using $\lambda=mn$ in (3). The discontinuity in this retention function is often referred to as the air entry or bubbling pressure point.

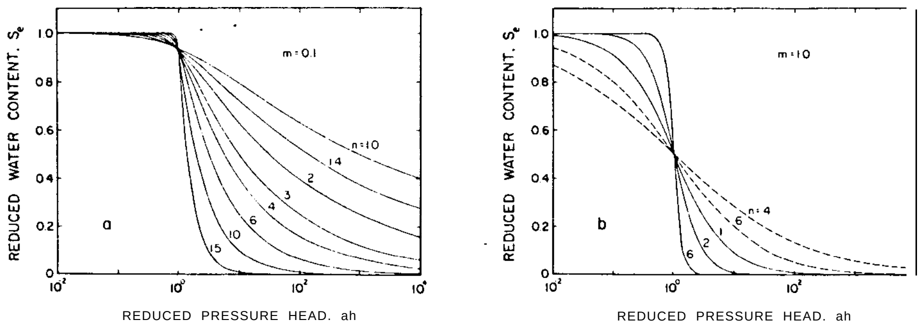


Fig. 1. Relationship between the reduced water content, $S_e=(\theta-\theta_r)/(\theta_s-\theta_r)$, and the reduced pressure bead, αh, according to the VG model for various values of and n, and (a) m=0.1 and *(b) m=1.* The S_e value for h = $1/\alpha$ is determined by m, whereas n is a measure of the slope of the retention curve.

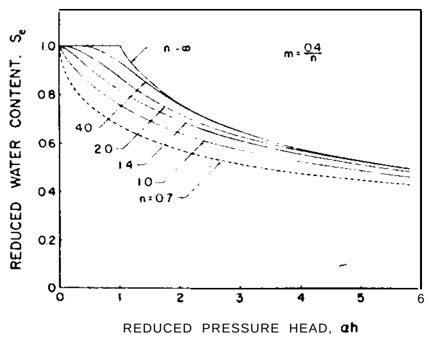


Fig. 2. Retention curves according to the VG model for various n, and mn=0.4. For $n\to\infty$, the limiting function is identical to the BC model with λ =mn.. In RETC we will use m = 1 and n = λ for the BC model.

Conductivity models

Although many predictive models exist for the hydraulic conductivity [cf. Mualem, 1986], the models by Burdine [1953] and Mualem [1976a] seem the most promising for obtaining closed-form expressions for K in conjunction with the BC and VG retention functions. The Burdine and Mualem models are given by

$$K_r = S_e^l \frac{g(S_e)}{g(1)} \qquad \text{Burdine (BU)} \tag{5}$$

in which

$$g(S_e) = \int_0^{S_e} h^{-2}(x)dx$$

and

$$K_r = S_e^{\ell}\left[\frac{f(S_e)}{f(1)}\right]^2 \qquad \text{Mualem (MU)} \tag{6}$$

in which

$$f(S_e) = \int_0^{S_e} h^{-1}(x)dx$$

respectively, where K_r (= K/K_s) is the relative conductivity, and ℓ is a model parameter frequently taken equal to be 2 for the BU model and 0.5 for the MU model. Our experience suggests that ℓ may deviate significantly from these values for certain soils.

Substitution of the BC function $(\lambda = n)$ in these two conductivity models yields the following closed-form relationships for the hydraulic conductivity:

$$K_r = S_e^{\ell+1+2/n} \qquad \text{(BU)} \tag{7}$$

$$K_r = S_e^{\ell+2+2/n} \qquad \text{(MU)} \tag{8}$$

If we use the VG function to describe the water retention curve, we obtain

$$K_r = S_e^{\ell}\, \mathrm{I}_{\zeta}(r,s) \qquad (\zeta = S_e^{1/m};\ r = m + 2/n;\ s = 1 - 2/n;\ n \geq 2) \qquad \text{(BU)} \tag{9}$$

$$K_r = S_e^{\ell}\, [\mathrm{I}_{\zeta}(p,q)]^2 \qquad (\zeta = S_e^{1/m};\ p = m + 1/n;\ s = 1 - 1/n;\ n \geq 61) \qquad \text{(MU)} \tag{10}$$

where I_ζ as the incomplete beta function. For most values of S_e, RETC evaluates this function with continued fractions according to:

$$\mathrm{I}_{\zeta}(x,y) = \frac{\zeta^x (1-\zeta)^y}{x\, \mathrm{B}(x,y)} \left[1/(1 + d_1/(1 + d_2/...))\right] \tag{11}$$

with

$$d_{2m+1} = -\frac{(x+m)(x+y+m)}{(x+2m)(x+2m+1)}\,\zeta \tag{12a}$$

$$d_{2m} = \frac{m(y-m)}{(x+2m-1)(x+2m)}\,\zeta \tag{12b}$$

Figures 3 and 4 show conductivity curves based on the VG functions using the BU and MU prediction models, respectively, for various n values, with mn fiied at 0.4. Notice the restriction $n>2$ for the BU model and $n>1$ for the MU model. This is because the incomplete beta function B(x,y) approaches infinity when n-2 for the BU model, or when n-l for the MU model. The MU model is therefore preferable since it can be applied to more soils than the BU model.

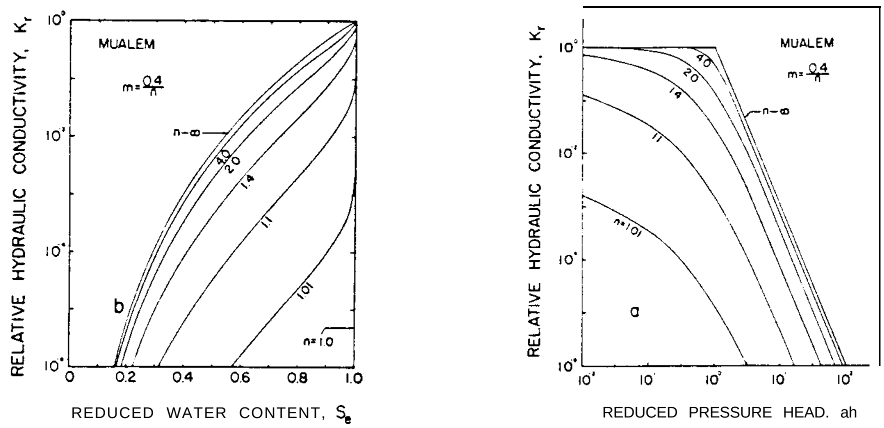


Fig. 3. Calculated curves for the relative hydraulic conductivity versus reduced pressure head (a) or reduced water content ***(b) as*** predicted from the retention curves of Figure 2, using Burdine's model.

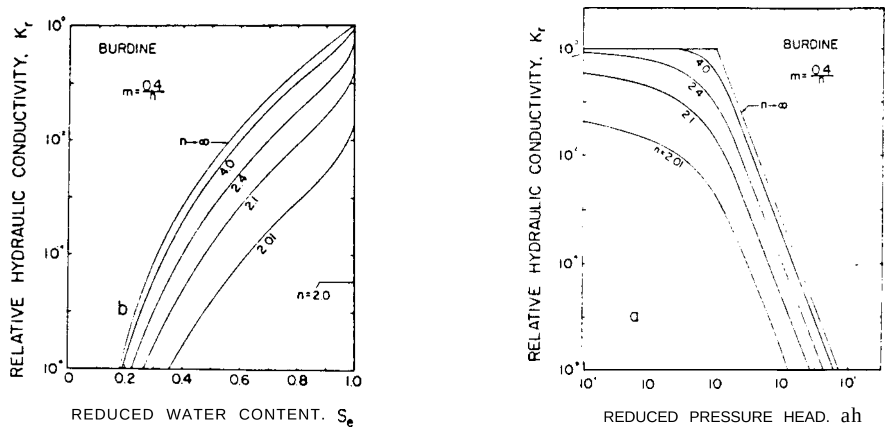


Fig. 4. Calculated curves for the relative hydraulic conductivity versus reduced pressure head (a) or reduced water content ***(b) as*** predicted from the retention curves of Figure 2, using Mualem's model.

Simpler expressions arise for the VG based models if the permissible values for m and n are restricted:

$$K_r = S_e^{\ell}\left[1-(1-S_e^{1/m})^m\right] \qquad (m=1-2/n;\, 0<m<1) \quad (\mathrm{BU}) \tag{13}$$

$$K_r = S_e^{\ell}\left[1-(1-S_e^{1/m})^m\right]^2 \qquad (m=1-1/n;\, 0<m<1) \quad (\mathrm{MU}) \tag{14}$$

Note that expressions for the soil-water diffusivity, D, can be readily derived from C, by differentiating the appropriate expression for the retention function, and using the selected function for *K*.

RETC: ANALYSIS OF RETENTION AND CONDUCTIVITY DATA

Parameter Estimation

The objective function, **O(b),** to be minimized in RETC, is written as a weighted least-squares type expression [cf., *Kool et al.,* 1987]:

$$\min_{\mathbf{b}} O(\mathbf{b}) = \sum_{i=1}^{N}\left[w_i\left(\theta_i - \hat{\theta}_i(\mathbf{b})\right)\right]^2 + \sum_{i=N+1}^{M}\left[w_i W_1 W_2\left(Y_i - \hat{Y}_i(\mathbf{b})\right)\right]^2 \tag{15}$$

where θ_i and $\hat{\theta}_i$ are the observed and fitted water contents, respectively, Y_i and $\hat{Y}_i$ are the observed and fitted conductivity or diffusivity data, N is the number of retention data points, M is the total number of observed data points (i.e., *M-N* denotes the number of conductivity/diffusivity data), w_i are weighing factors for the individual data points, and W_1 and W_2 are additional weighing factors in the conductivity/diffusivity term as defined below. The trial parameter vector, $\mathbf{b} = (\theta_r, \theta_s, \alpha,$ n, m, $\ell, K_s)^T$, *in* (16) contains the unknown model parameters to be fitted to the data. The parameters are estimated with an algorithm described by ***Marquardt*** [1963].

The weights w_i in (15) are used to express the reliability of each measurement, they are equal to the inverse of the observation error. Generally no reliable estimates for individual observation errors are available, and it is often assumed that $w_i = 1$ for all *i* (ordinary least-squares method). The RETC code assumes $w_i = 1$, unless specified otherwise by the user. The parameter W_2 is calculated internally in the program according to

$$W_2 = \frac{(M-N)\sum_{i=1}^{N} w_i\theta_i}{N\sum_{i=N+1}^{M} w_i|Y_i|} \tag{16}$$

This parameter accounts for differences in the number of measurements and units. In addition, the parameter W_1 can be used by the user to give more or less weight of conductivity/diffusivity with respect to retention data as a whole. Having this feature is sometimes useful since conductivity or diffusivity are often less reliable than retention data.

Because the observation error generally depends on the magnitude of the observation, the ‘assumption that $w_i = 1$ is not correct. This is particularly true for conductivity/diffusivity data, where the largest and smallest observation may differ several orders of magnitude. RETC has the option of implementing a logarithmic transformation to partially remedy this problem.

Program Options

RETC can be used for a combination of descriptive and predictive problems as specified by the program variables MIT and KWATER. The following broad categories can be distinguished:

1. Hydraulic functions can be predicted from known prescribed model parameters (MIT=0, or if M=N=0).
2. Experimentally determined points for $\theta(h)$ and K or D can be fitted simultaneously if both retention and conductivity or diffusivity data are available (KWATER=O).
3. Experimental data points for $\theta(h)$ can be fitted, and K or D predicted (KWATER = 1).
4. Observed K- or D-values can be fitted, and $\theta(h)$ predicted (KWATER=2).

The program can simultaneously fit all model parameters. This procedure appears to give better results than successively fitting $\theta(h)$ and K to the experimental data [Yates et *al.,* 1992]. RETC has the flexibility to estimate one, several, or all unknown parameters within one of the above estimation categories. However, the parameter estimation procedure is generally improved if the number of unknown parameters is reduced.

Program variables may be selected as shown in Tables 1 and 2. The choice of a particular retention and conductivity model is governed by the variable MTYPE. Table 1 lists the various options for this variable.

The input parameter METHOD is used to specify the type of conductivity or diffusivity data used in the optimization process; both original or log-transformed data can be fitted/predicted and the independent variable for K can either be θ or h. Table 2 shows the settings of METHOD

TABLE 1. Available Retention and Conductivity Models in RETC

MTYPE	Retention Function	Conductivity Model
1	van Genuchten	Mualem
2	van Genuchten	Burdine
3	van Genuchten (m = l-l/n)	Mualem
4	van Genuchten $(m = 1\text{-}2/n)$	Burdine
5	Brooks-Corey	Mualem
6	Brooks-Corey	Burdine

TABLE 2. Selection of METHOD for Possible Lop-transformation of Data

METHOD	1	2	3	4	5	6
Type of *K/D* data	$K(\theta)$	log $K(\theta)$	$K(h)$	log $K(h)$	$D(\theta)$	log $D(\theta)$

Recommendations for Program Use

Except for well-defined data sets with observations covering a wide range of water content and/or conductivity/diffusivity data, it is recommended that the number of parameters be limited as much as possible. Some suggestions are given below:

1. For reasonably well-defined data sets, run the program first with all six (MTYPE=3,4) or seven (MTYPE = 1, 2) parameters as unknowns. The output always includes a correlation matrix for the unknown coefficients. Some of the parameters are sometimes highly correlated, the most frequent case being ***between*** ℓ and n (and/or ***m if*** MTYPE= 1 or ***2).*** If the correlation coefficient between those two coefficients exceeds 0.95 or 0.98, it might be better to fix the exponent ℓ at some convenient value, preferably at 0.5 for Mualem's model and 2.0 for Burdine's model, unless the previously fitted value deviates significantly from these averages.

2. Use MTYPE=3, unless the observed data show little scatter and cover a wide range of pressure head and/or hydraulic conductivity data. It is not likely that the restriction imposed by MTYPE=3 (Mualem's model with m = l-l/n) will greatly compromise the accuracy of the fit if field soils are analyzed [van Genuchten ***and Nielsen, 1985].***

3. Fix the conductivity at saturation, K_s, only if a good estimate is available. Sometimes an accurate estimate for ***K*** (or D) is available at a point less than saturation. If that data point is judged to be more accurate than others, give it more weight by increasing the value of the weighing coefficient w_i for that data point (i.e., $w_i = 3$, 5 or larger).

4. Routinely rerun the program with different initial estimates to make sure that the program converges to approximately the same final parameter values.

Example

To illustrate results obtained with the RETC program, we used measured data for a Weld silty clay loam reported by Mualem [1976b]. In this example, the variable MTYPE is set to 3, and METHOD equal to 2. Figure 5 compares experimental retention points with the theoretical curve fitted to these data using the VG model with $m = 1-1/n$. The fitted values for θ_r, θ_s, α, and n as obtained with RETC are shown in the figure. Figure 6 compares the experimental conductivity values and the curve "predicted according to Mualem's model using the values listed in Figure 5, and assuming $\ell = 0.5$ and $K_s = 1$. Notice that the model under-predicts the observed conductivity data. Figure 7 compares the same conductivity data with a calculated curve obtained by simultaneously fitting the VG-Mualem models to observed retention and conductivity data, assuming as before that $\ell = 0.5$ and $K_s = 1$. In this case the fitted curve corresponds much better to the experimental data.

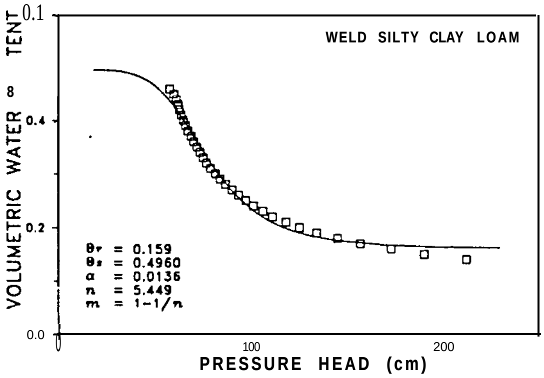


Fig. 5. Fit of the VG function to water retention data.

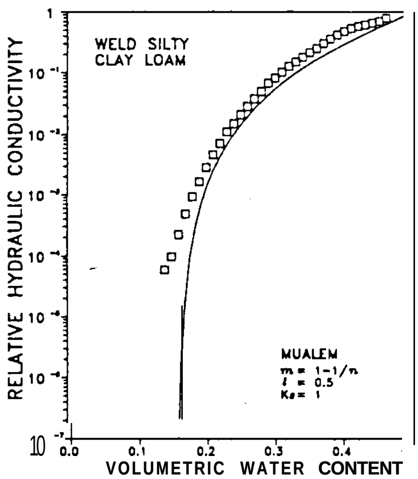
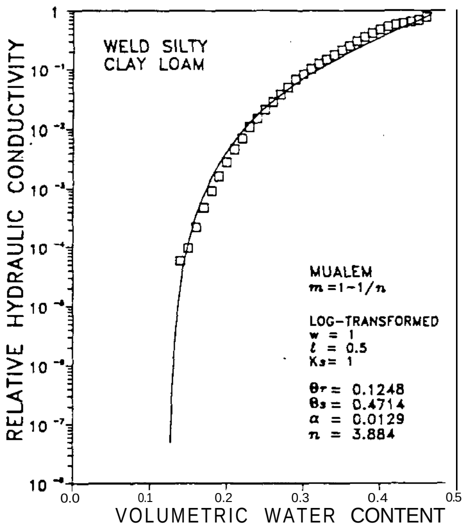


Fig. 6. Hydraulic conductivity predicted with the MU model using parameter estimates from Figure 5.

SUMMARY AND CONCLUSIONS

This paper reviews expressions for the retention curve according to Brooks-Corey and van Genuchten, and predictive equations for the hydraulic conductivity curve according to Mualem and Burdine. It is shown how these models can be combined to yield sets of hydraulic functions for predicting retention and conductivity or diffusivity curves assuming known model parameters. Alternatively, values for the parameters can be estimated by fitting the hydraulic models to experimental data using the RETC code. A brief description of the parameter estimation procedure is given, explaining the need for using weighing factors and transformed variables. An example shows that the hydraulic conductivity curve can be predicted using parameters fitted to observed retention data, or using parameters obtained from a simultaneous fit to observed retention and hydraulic conductivity data.



Fii. 7. Hydraulic conductivity according to the VG and MU models fitted simultaneously to the retention and conductivity data.

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