MODELS TO PREDICT UNSATURATED HYDRAULIC CONDUCTIVITY WITH THE USE OF RETC CODE Ali J. Kadhim

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ABSTRACT

The soil hydraulic characteristics , the soil water content and unsaturated hydraulic conductivity are essential to many agriculture and environmental applications. There are many important methods to estimate the soil water content and unsaturated hydraulic conductivity (K), and used this technique to predict the equation parameters (θ r , θ s , α ,m ,n). Three models(van Genuchten – Mualem m= 1-1/n , van Genuchten – Burdine m=1-2/n and Brooks & Corey $n\rightarrow\infty$) were fitted with soil moisture retention data using RETC Code .The RETC code was developed at US salinity laboratory and it used world –wide in many papers at now. Method this program allows to compare three models from the input of moisture retention curve data. In this study , calculated three relationship water content vs pressure head , relative unsaturated hydraulic conductivity with water content and pressure head respectively .And , used various closed – form analytical models for predicting the hydraulic conductivity. Van – Genuchten derived equation Mualem (1976) with a new model for predicting from the soil water retention curve . Equation Mualem's derivation leads to a simple integral formula for predicting the unsaturated hydraulic conductivity. The three model gave an excellent description of soil moisture data with van Genuchten , Mualem model (m=1-1/n) being superior over the other models having the highest coefficient of determination R2 =0.9843 and lowest sum of squares of residual SSQ = 0.0031.

كاظم

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نماذج للتنبؤ بالايصالية المائية غير المشبعة باستخدام برنامجRETC علي جواد كاظم كلية الزراعة – جامعة واسط

المستخلص

تعد الخصائص المائية للتربة ، المحتوى الرطوبي للتربة والإيصالية المائية غير المشبعة اساسية للكثير من التطبيقات الزراعية والبيئية . وتوجد الكثير من الطرق المهمة لتقدير منحى المحتوى الرطوبي والايصالية المائية غير المشبعة واستخدمت هذه التقنية للتنبؤ عن ثوابت المعادلة .(θr, θs, α, m, n) تم مطابقة ثلاثة نماذج رياضية no (θr, θs, α, m, n) و – Van Genuchten – Mualem m=1-1/ و (θr, θs, α, m, n) و المعادلة .(θr, θs, α, m, n) و المعادلة نماذج رياضية Brooks & Corey n و (θr, θs, α, m, n) و المعادلة . و Burdine m=1-2/n و (∞ – m) و (θr, θs, α, m, n) و المعادلة منحنى الوصف الرطوبي باستخدام برنامج . ETC وان برنامج المعادلة .(βs, α, m, n) تقدر من قبل مختبر الملوحة الأمريكي واستخدم على مدى واسع في كثير من البحوث لحد الأن .ان هذا البرنامج يسمح بالمقارنة الثلاثة نماذج من خلال ادخال بيانات منحنى الوصف الرطوبي . في هذه الدراسة ، تم حساب ثلاثة علاقات : المحتوى الرطوبي مع الشد ، الإيصالية المائية غير المشبعة النسبية مع الرطوبة والشد على الترتيب .واستخدمت صيغ تحليلية مغلقة مختلفة للتنبؤ عن الإيصالية المائية غير المشبعة .اشتق المائية غير المشبعة النسبية مع الرطوبي . في هذه الدراسة ، تم حساب ثلاثة علاقات : المحتوى الرطوبي مع الشد ، عزر المشبعة .اشتق معادلة المائية على الترتيب .واستخدمت صيغ تحليلية مغلقة مختلفة للتنبؤ عن الايصالية المائية المائية عن الايصالية المائية من المائية المائية معالمة المائية عن المائية من خلال منحى رطوبة التربة.حيث قاد اشتقاق معادلة (Mulean الى ضيغة عدية بسيطة للتنبؤ عن الايصالية المائية غير المشبعة. لقد اعطت منحى رطوبة التربة.حيث قاد اشتقاق معادلة (Mulean الى ضيغة عدية بسيطة للتنبؤ عن الايصالية المائية غير المشبعة من خلال منحى رطوبة التربة.حيث قاد اشتقاق معادلة (Mulean الى ضيغة عدية بسيطة للتنبؤ عن الايصالية المائية غير المشبعة من خلال منحى رطوبة المربعة المائية ممانية ممادلة (Mulean الى ضيغة عدية بسيطة التنبؤ عن الايصالية المائية غير المشبعة. المتوقة منحى رطوبة المربعة المائية ممادلة (Mulean الى ضيغة عدية بسيطة التنبؤ عن الايصالية المائية على المشبعة. المتومة منحن محلال المائية المائية عبر المشبعة المنوقة النداذج الرياضية المائيا المائية ممادلة (Genuchten , Mualem (m=1-1/n) المحوي مائية مادخلال المائيا المالما

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INTRODUCTION

Computer models are now routinely used in research and management to predict the movement of water and chemicals into and through the unsaturated zone of soils . Accurate in situ measurement of the unsaturated hydraulic conductivity has remained especially cumbersome and time-consuming. Measured input retention data may be given either in tabular form, or by means of closed-form analytical expressions which contain parameters that are fitted to the observed data. In a porous system, increasing the value of suction ψ (defined by ua-uw, where ua is the air pressure and uw is the reduce water pressure) tends to θ [Germann, 7]. The quantity of water retained in a soil by suction depends on many factors, namely: shape, size and distribution of pore space ;mineralogy and surface activity of solid grain particles; and the chemical composition of interstitial water. The desaturation is typically more pronounced in coarsegrained materials (such as sand and gravel) than in fine-grained materials (such as silt and clay). The value of θ at a given ψ also depends on the path, whether it occurs during a wetting or drying phase. Different paths may induce somewhat different curves, but such hysteresis phenomena will not be addressed directly herein, as only the drainage path is considered here (to simplify the presentation). In this study, projected data were used three soils to determine water retention curve . The RETC Code program may be used to fit several analytical models to observed water retention and/or unsaturated hydraulic conductivity data. The RETC code is a descendent of the SOHYP code previously documented by van

Genuchten [21].As before, soil water retention data are described with the equations of Brooks and Corey [2] and van Genuchten [22], whereas the poresize distribution models of Burdine [3] and Mualem [16] are used to predict the unsaturated hydraulic conductivity function. New features in RETC include (1) a direct evaluation of the hydraulic functions when the model parameters are known,(2) a more flexible choice of hydraulic parameters to be included in the parameter optimization process, and (3) the possibility of evaluating the parameters model from observed conductivity data rather than only from retention data, or simultaneously from retention and measured hydraulic conductivity data. Although the models used in RETC is intended to describe the unsaturated soil hydraulic properties for drving wetting monotonic or in homogeneous soils, the code can be easily modified to account for more complicated flow processes such as hysteretic two-phase flow Lenhard et al., [11] or preferential flow [Germann, 7]. The objectives of this study to comprise three retention curve. RETC Code The purpose of this report is to document the RETC (RETention Curve) computer program for describing the hydraulic properties of unsaturated soils.

Theorical Consideration Soil Water Retention Models

Several functions have been proposed to empirically describe the soil water retention curve. One of the most popular functions has been the equation of Brook and Corey [2], further referred to as the BC-equation:

where θr , and θs , are the residual and saturated water contents, respectively; α is an empirical parameter (L-l) whose inverse is often referred to as the air entry value or bubbling pressure, and λ is pore-size distribution parameter а affecting the slope of the retention function. For notational convenience, h and a for the remainder of this report are taken positive for unsaturated soils (i.e., h denotes suction). The residual water content, θr in Eq. (1) specifies the maximum amount of water in a soil that will not contribute to liquid flow because of blockage from the flow paths or strong adsorption onto the solid phase [Luckner et al., 13]. Formally, θr may be defined as the water content at which both $d\theta/dh$ and K go to zero when h becomes large. The residual water content is an extrapolated parameter, and hence may not necessarily represent the

smallest possible water content in a soil. This is especially true for arid regions where vapor phase transport may dry out soils to water contents to well below θr The saturated water content. θs sometimes also referred to as the satiated water content, denotes the maximum volumetric water content of a soil. The saturated water content should not be equated to the porosity of soils; θ s of field soils is generally about 5 to 10% smaller than the porosity because of entrapped or dissolved air. Following Van Genuchten and Nielsen [23] and Luckner et al. [13], θ r and θ s, in this study are viewed as being essentially empirical constants in soil water retention functions of the type given by Eq. (1), and hence without much physical meaning.Equation (1) may be written in a dimensionless form as follows

$$Se = \begin{cases} (\alpha h)^{-\lambda} (\alpha h > 1) \\ 1 \ (\alpha h \le 1) \end{cases}(2)$$

where Se, is the effective degree of saturation, also called the reduced water content (0 < Se < 1):

On a logarithmic plot,Eq. (2) generates two straight lines which intersect at the air entry value, ha=l / a. Because of their simple form,Eq. (2) and (3) have been used in numerous unsaturated flow studies. The BC-equation has been shown to produce relatively accurate results for many coarse- textured soils characterized by relatively narrow poreor particle-size distributions (large Rvalues).Results have generally been less accurate for many fine-textured and undisturbed field soils because of the absence of a well-defined air-entry value for these soils. Several continuously differentiable (smooth) equations have been proposed to improve the description of soil water retention near saturation. These include functions introduced by King [8], Visser [25], Laliberte [10], Su and Brooks [20] and Clapp and Hornberger [4]. While these functions were able to reproduce observed soil water retention data more accurately, most are too complicated mathematically to be easily incorporated

$$Se = \frac{1}{[1 + (\alpha h)^n]^m}$$
(5)

where α , n and m are empirical constants affecting the shape of the retention curve. Equation (5) with m = 1 was used earlier by [Ahuja and Swartzendruber, 1], [Endelman et al., 6] and [Varallyay and Mironenko, 24], among others.

Mualem's Hydraulic Conductivity Model

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into predictive pore-size distribution models for the hydraulic conductivity, or possess other features (notably the lack of a simple inverse relationship) which make them less attractive in soil water studies [van Genuchten and Nielsen, 23]. A related smooth function with attractive properties is the equation of van Genuchten [22], further referred to as the VG-equation:

The model of [Mualem ,16] for predicting relative hydraulic the conductivity, K, [Burdine ,3] may be written in the form

Where

in which Se(sometime called effective saturation) is given by Eq. (6), K, is the hydraulic conductivity at saturation, and e is a pore-connectivity parameter estimated by Mualem [16] to be about 0.5 as an average for many soils. To facilitate the integration inEq. (7), we first take the inverse of Eq.(5) as follows

Substituting Eq.(8) into Eq.(7) and using the substitution x=ym gives

Several approaches can now be followed to derive K from Eq.(6) and Eq. (9). We first proceed with the most general case of variable m and n. The transformations

And

where B(p,q) is the Complete Beta function given by

and is the Incomplete Beta function Zelen and Severo, (29):

The simplest case arises when k=0, which leads to the restriction m = l-l/n. Equation (9) can now be readily integrated to yield

or in terms of the pressure head :

Burdine's Hydraulic Conductivity Model

The model of Burdine [3] can be written in a general form as follows

RETC

RETC (RETention Curve) uses a nonlinear least-squares optimization approach to estimate the unknown model parameters from observed retention and/or conductivity or diffusivity data. A helpful text with background information on fitting equations to experimental data using this method is given by [Daniel and Wood 5]. The approach is based on the partitioning of the total sum of squares of he observed values into a part described by the fitted equation and a residual part of observed values around those predicted with the model. The aim of the curve fitting process is to find an equation that maximizes the sum of squares associated with the model, while minimizing the residual sum of squares, SSQ. The residual sum of squares reflects the degree of bias (lack of fit) and the contribution of random errors. SSQ will be referred to as the objective function O(b) in which b represents the unknown parameter vector .The RETC minimizes O(b) iteratively by means of a weighted least-squares approach based on Marquardt's maximum neighborhood

When only retention data are used, the objective function is given by

where θi , and θi are the observed and fitted water contents, respectively, and N is the number of retention data points. The weighting coefficients, Wi in Eq. (18) may be used to assign more or less weight to a single data point depending upon a priori information. The wi's reflect the reliability of the measured data points, and ideally should be set equal to the inverse of the observation errors (i.e., the standard deviation) which account for sampling and experimental errors. It can be shown that for the correct weights, the variances of all elements bj of b are minimized simultaneously [Daniel and Wood, 5]. Unfortunately, reliable estimates of the

observation of individual errors measurements are generally lacking. Because of this the wi are often set to unity. If all observation errors are normally distributed, possess a constant variance, and are uncorrelated, wi= 1 for all i and the optimization method reduces to the ordinary least-squares method Kool et al., [9]. The optimization procedure becomes more complicated when the unknown parameter vector b is fitted simultaneously to observed retention and hydraulic conductivity or soil water diffusivity data. The objective function to be minimized in RETC is then of the general form

$$O(b) = \sum_{i=1}^{N} \{ w_i [\theta_i - \theta_i(b)] \}^2 + \sum_{i=N+1}^{M} \{ W_i W_1 W_2 [(Y_i - \hat{Y}_i)(b)] \}^2 \dots \dots \dots \dots (19)$$

where Yi and Yi are the observed and fitted conductivity or diffusivity data, W1 and W2 are weighting factors as explained below, and M is the total number of observed retention and conductivity or diffusivity data points. The parameter W2 is introduced to ensure that proportional weight is given to the two different types of data in Eq.(19), (i.e., W2 corrects for the difference in number of data points and also eliminates, to some extent, the effect of having different units for B and

| K or D). | The value for W2 is calculated | internally in the program according to |
|-------------------------|---|--|
| W ₂ = | $\frac{(M-N)\sum_{i=1}^{N}W_{i}\theta_{i}}{N\sum_{i=N+1}^{M}W_{i} Y_{i} }\dots$ | |

The effect of Eq.(20) is to prevent one data type in Eq.(19) (usually the K or D data) from dominating the other data solely because of its larger numerical values. The weighting factor W1 is included in Eq. (19) to add extra flexibility to the parameter optimization process. The W1 allows one to place more or less weight on the hydraulic conductivity data in their entirety, relative to the soil water retention data. Because conductivity data usually show considerably more scatter than water content data, and generally are also less precise, it is often beneficial to assign relatively less weight to the conductivity data in Eq.(20). This may be accomplished by using a value of less than 1 for W1. Recent studies with RETC [Wösten and van Genuchten, (27); Sisson and van Genuchten, (19); Yates et al., (28)] have successfully used values between 0.1 and 1.0 for W1,. Assigning wi= 1 to all data points assumes that the observation errors for a particular variable are all very similar and independent of the magnitude of the measured data. This is clearly not true for most hydraulic conductivity and diffusivity data sets where the largest and smallest observations can easily differ several orders of magnitude. The resulting errors can be kept to a minimum by applying a logarithmic transformation to the K or D data prior to the parameter estimation process. RETC has the option of implementing a logarithmic transformation of K/D by using y=log(Ki) or yi=log(Di) in Eq.(19)

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before carrying out the parameter estimation process. We recommend the use of a logarithmic transformation unless special accuracy of the conductivity or diffusivity function in the wet range is required. In that case one may decide to use the untransformed data since these put relatively more weight on the higher K and D values. The unsaturated soil hydraulic functions contain up to 7 unknown independent parameters. Except for well-defined data sets covering a wide range of 8 and/or K/D data, it is important to limit as much as possible7 the number of parameters to included be in the parameter optimization process. Limiting the number of fitting parameters is especially important for in situ field data sets which often are poorly defined and may contain relatively large observation errors. Unbalanced data sets with many poorly defined (scattered) data over a limited range of water contents (or conductivities/diffusivities) inevitably lead to parameter uniqueness problems, exemplified by poor convergence and large confidence intervals for the parameter estimates. By comparison, a few (e.g., 6 to 10) well-placed retention data covering a wide range in water contents may lead to rapid convergence relatively narrow confidence and intervals. Several suggestions for limiting the number of parameters are given below. We refer to the text by Daniel and Wood [5] for a more detailed general discussion of disposition of data points. The RETC output always

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includes a matrix which specifies degree between of correlation the fitted coefficients in the different hydraulic models. The correlation matrix quantifies the change in model predictions obtained with a new estimate for a particular parameter relative to similar changes as a result of new estimates for the other parameters. The matrix reflects the nonorthogonality between two parameter values. A value of \pm 1 suggests a perfect linear correlation whereas 0 indicates no correlation at all. We suggest to always а "backward" type perform of regression, i.e., by initially fitting all parameters and then fixing certain one if these parameters one by parameters exhibit high correlations. Hence, for well-defined data sets it is usually best to first keep all 6 (for restricted m and n) or 7 (for variable

m,n) parameters as unknowns when a simultaneous fit is carried out. The correlation matrix may be used to select which parameters, if any, are best kept constant in the parameter estimation process because of high correlation. The most frequent cases of correlation occur between m, n and if no restrictions are placed on m and n, and between n and if one of the restrictions on m and n is imposed. If the correlation between n and exceeds 0.98 or 0.99, we suggest to fix the exponent at some convenient value, preferably at 0.5 for Mualem's model and 2.0 for Burdine's model, unless the previously fitted value significantly from deviates these averages. Another important measure of the goodness of fit is the value for regression of the observed, ŷi, versus fitted, y,(b), values :

The value is a measure of the relative magnitude of the total sum of squares associated with the fitted equation; a value of 1 indicates a perfect correlation between the fitted and observed values. The RETC provides additional statistical information about the fitted parameters such as mean, standard error, T-value, and lower and upper confidence limits. The standard error, S(bj), is estimated from knowledge of the objective function, the number of observations, the number of unknown parameters to be fitted, and an inverse matrix [Daniel and Wood, 5].

Materials and Methods

The data were selected from Al – Jaderiah soil , sandy loam .The soil texture were determinate (741.4 , 190.3 and 68.3) gm / kg sand , silt and clay respectively .Disturbed surface sample (0 - 30) cm were passed through a 2 – mm sieve .The Moisture curve were calculated with use pressure plate , then predicted the unsaturated hydraulic conductivity , and compare with three models in table (1).

RETC Code

relative unsaturated hydraulic conductivity.

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Use the program RETC Code (Retention Curve)Version 6.0 to predict on the

| М Туре | Retention Model | Conductivity Model |
|--------|------------------------------------|--------------------|
| 1 | Eq.(5) with $m=1-1/n$ | Maulem's (Eq.7) |
| 2 | Eq.(5) with $m=1-2/n$ | Burdin's (Eq.7) |
| 3 | Eq.(1) with $n \rightarrow \infty$ | Maulem's (Eq.7) |

Table 1. Type of retention and conductivity models implemented in RETC as afunction of the input variable MTYPE (Method Type)

Results and Discussion

1. Calculation of soil water retention curve

Figure (1) show typical calculated retention curve based on Eq.(5) for various of m and n. Plots are given using semi – logarithmic scale for the reduced pressure head (αh) . The curves in Figure (1A,1B,1C) for three models Van Genuchten – Mualem , m= 1-1/n , Van Genuchten – Burdine , m=1-2/nand Brooks & Corey, $n \rightarrow \infty$ respectively. As shown in Figure (1), that leads to a sharp break in the curve at the air entry. Smooth curves with less or more segmoidel shaped on semi – logarithmic plots were obtained when n is allowed to hold finite value. In all model, in Figures (1A,2B,3C) the retention curve approach saturation with a zero slop only when $\alpha > 1$ [van Genuchten and Nielson , 1985]. Figures also demonstrate the effects on the curves when various restriction are placed on permissible value of m and n . When $n \rightarrow \infty$, the limiting curve of Brooks & Coery (1964) with a well - defined air entry value appears. When m=1-1/n as used by Van Genuchten (1980) for the Mualem based conductivity prediction . Similarly

, when m=1-2/n for Burdine - based conductivity equation of Van Genuchten (1980) [Salem, (18), Matula et.al.(15)]. We emphasize here that Eq.(5) contain five independent parameters (θ s, θ r, α , m. n) and that the residual and saturated water contents are considered here to be empirical parameters. They are defined the retention model , and fitted to observed data using that retention models. Of the three remaining parameters, α approximately equals the inverse of the air entry value for small m/ n values, while for large m/n this parameter roughly equals the inverse of the pressure head at the inflection point $(\theta - \Psi)$ curves. The product mn determines the slop of the curve at large value of the suction head and hence mostly affected by soil texture, while soil structure effected usually appears near saturation Wildenschild et al.(26). To verify the ability of Eq.(5) in matching experimental data, a non – liner least optimization method analogous to that described by Van Genuchten (1978) .RETC was used to analyze numerous published $(\theta - \Psi)$ data set. Fitted values for the parameters are given in table (2) indicates that the restricted case, m=1-1n







Figure (1): Relationship between suction head and water content for three equation A (m=1-1/n) , B(m=1-2/n) and C (n $\rightarrow\infty$).

| Soil texture | Type of curve | θr | θs | α | n | m | R2 | SSQ |
|-----------------|------------------|--------|--------|--------|--------|--------|--------|--------|
| Loamy sand | m=1-1/n | 0.0780 | 0.4300 | 0.0360 | 1.5600 | 0.3590 | 0.9843 | 0.0031 |
| | m=1-2/n | 0.0780 | 0.4300 | 0.0360 | 2.0500 | 0.2440 | 0.9831 | 0.0033 |
| | n→∞ | 0.0780 | 0.4300 | 0.0360 | 1.5600 | 1 | 0.9790 | 0.0041 |

| Table (2): | Fitting values | or parameters in | equation (5) |) for retention curves |
|-------------------|----------------|------------------|--------------|------------------------|
|-------------------|----------------|------------------|--------------|------------------------|

produced the best fit as it shows values of the residual sum of Square (SSQ) and the coefficient of determination (R2). Fitted parameter values given in table (2) are used to illustrate the results of the observed and fitted retention for the soil . The hydraulic parameters listed in table (2) provide an excellent description of the soil water retention relationship Lu et al.(12).

2. Prediction of the Hydraulic conductivity

Figure (2) and (3) show calculated curves of the prediction relative hydraulic conductivity as a function of both the suction head (α h) and the water content Kr(θ). The prediction curves are obtained from fitting the hydraulic parameters of the restricted case gives an excellent prediction for relative hydraulic conductivity but the function

seems to under estimate the relative hydraulic conductivity at high water content values Priesack & Durner (17). curve of the relative Prediction hydraulic conductivity as a function of suction head, $Kr(\Psi)$, for the restricted case is shown in figure (2). The predition curve was obtained from fitting the hydraulic conductivity parameters of the retention curve, which is given in figure (3). Figures (2) and (3) show that the relativr hydraulic conductivity curve decrease in value when n unity, because of the complete Beta function B(p,q)goes to infinity when $n \rightarrow 1$. Conclusion This article has shown that Eq. (5) gave excellent fitting for the retention curves data for the three models, where van Genuchten – Mualem equation m=1-1/nwas being the best in terms of fitting in comparison with other two models. This model showed a very good results in prediction

| Soil texture | Type of curve | θr | θs | α | n | m | R2 | SSQ |
|-----------------|------------------|--------|--------|--------|--------|--------|--------|--------|
| Loamy sand | m=1-1/n | 0.0780 | 0.4300 | 0.0360 | 1.5600 | 0.3590 | 0.9843 | 0.0031 |
| | m=1-2/n | 0.0780 | 0.4300 | 0.0360 | 2.0500 | 0.2440 | 0.9831 | 0.0033 |
| | n→∞ | 0.0780 | 0.4300 | 0.0360 | 1.5600 | 1 | 0.9790 | 0.0041 |

Table (3): Relationship between water content and relative unsaturated hydraulic conductivity for three equation A (m=1-1/n), B (m=1-2/n) and C ($n \rightarrow \infty$).







Figure (2): Relationship between suction head and relative unsaturated hydraulic conductivity for three equation A (m=1-1/n) , B (m=1-2/n) and C ($n \rightarrow \infty$).

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