Calibration of van Genuchten Unsaturated Hydraulic Conductivity Parameters by Regression Technique

Turgut Kutlu^{1,*}, Sabit Ersahin²

^{1,} Arslanbey Vocational School, Kocaeli University, 41285 Kocaeli-Turkey. ^{*}E mail: turgut.kutlu@kocaeli.edu.tr ²Department of Soil Science, Agricultural Faculty, Gaziosmanpasa University 60250 Tokat-Turkey

ABSTRACT

Unsaturated hydraulic conductivity is the mainstay, modulating water and chemical transport in the field. Measurements of parameters take place in the processes are difficult and require time, labor and finance. Thus, correct estimation of these parameters is very important to save valuable sources. The purposes of the study was to estimate van Genuchten unsaturated hydraulic conductivity parameters with RETC-ROSETTA program and calibrating the estimations by regression technique using easily measured soil physical properties, such as components of texture, bulk density and water holding capacity. Total, 168 soil and bulk density samples were collected from 0-30 cm soil depth in an alluvial area located over young river terraces of Yesilırmak near Tokat city. The soil samples were analyzed for clay, silt, sand, and organic matter, and saturated hydraulic conductivities of each sample was measured. Soil water content of each soil sample was determined for -10, -20, -33, -50, -75, -100, -300, -500, -700 and -1000 KPa soil water pressure. van Genuchten's water retention curve parameters, **a** and **n** parameters using RETC program, regression technique was used to develop equations to predict **a** and **n** parameters using basic soil parameters. Performance of regression-model was judged by correlation of estimations with observed values of validation data set.

Keywords: RETC, van Genuchten parameters, water retention curve, unsaturated hydraulic conductivity, estimation, modeling.

INTRODUCTION

Significant events such as runoff, drainage, soil reclamation, and chemical transport are related to unsaturated water transport, and this requires advanced knowledge of water flux under unsaturated conditions and spatial variation of this flux. Especially contaminant transport under unsaturated conditions is affected by soil hydraulic and chemical properties and process in soil (Thomasson and Wierenga, 2003). Numerical expression of water transport is difficult due to the variable moisture conditions through the soil profile. Hence, quantification is vitally important to model hydrological processes in soil system (Harter and Yeh, 1998; Tuli et al., 2001; Tartakovsky et al., 2003). Among soil hydraulic parameters, saturated hydraulic conductivity (Ks), and unsaturated hydraulic conductivity [Kus(θ)] or [Kus(ψ)] are most important ones. Measurement of these parameters requires time and intensive labor, and, is hence expensive. Thus, instead of measurement of soil hydraulic parameters scientist focused on the estimation of hydraulic parameters using routinely measured simple soil parameters such as textural components, bulk density, soil moisture, and

saturated hydraulic conductivity (Kosugi et al., 1997; Wagner et al., 1998; Zhuang et al., 2001; Schaap and Leij 2000). Many scientist have tried to relate (θ) to (ψ) and /or (K) to (ψ) by analyzing data of water movement under unsaturated conditions. (Kosugi at al., 1997).

One of the widely used water retention equation developed by van Genuchten (1980) is,

$$Se = \frac{1}{\left[1 + \left(\alpha h\right)^n\right]^{1-1/n}} = \left[1 + \left(\alpha h\right)^n\right]^{-m}$$
⁽¹⁾

Here, **h** is soil water pressure (cm); α (cm⁻¹), **n** and **m** are curve shape parameters of water retention. The parameter α is described as inverse of the pressure head at the point, where d θ /dh is maximum or as inverse of air entry value. The dimensionless van Genuchten's parameter n refers to the steepness of the water retention curve. **Se** is the effective saturation that relates volumetric water content for any d θ /dh to residual and saturated water content (θ , θ r, θ s) (cm³ cm⁻³) and expressed as,

$$S_e = (\theta - \theta_r) / (\theta_s - \theta_r)$$
⁽²⁾

Residual water content θ_r represents the soil water content at some large negative value of the soil water pressure head. Combination of Equation (1) and Muallem's (1976) particle size distribution model, results equation (3) to estimate unsaturated hydraulic conductivity (van Genuchten, 1980; Scaap, 1998);

$$K(Se) = Ks Se^{\lambda} \left[1 - \left(1 - Se^{1/m} \right)^m \right]^2$$
(3)

In equation (3), K(Se) and Ks are unsaturated and saturated hydraulic conductivity, and λ is an empiric constant usually accounted as 0.5 (Muallem, 1976), and m is equal to 1-1/n. By using equation (3), van Genuchten et al., (1991) developed RETC (**RET**ention Curve) computer model to estimate unsaturated hydraulic conductivity using hierarchical application of soil parameters.

The aims of this study were to estimate van Genuchten's water retention parameters α and n with easily measured soil physical properties using RETC computer program, and (ii) to calibrate estimated α and n parameters to increase estimation validity.

MATERIAL and METHODS:

Sampling and Soil Analysis

For this study, total 168 soil samples taken from 0-30 cm depth were analyzed for texture components (SSiCl) (%) (Gee and Bauder, 1986), bulk densities (BD) (gr cm⁻³) (Blake and Hartage, 1986), saturated hydraulic conductivity (K) (cm day⁻¹) (Klute and Dirksen, 1986), and water retention curve (Klute, 1986). For water retention curve, volumetric water content measured for -10, -20, -33, - 50, -75, -100, -300, -500, -700, and -1000 KPa soil water pressure. Saturated water content was obtained by curve fitting of retention data. Data of texture class and components (SSiCl) (Sand, Silt and Clay), SSiCl + Bulk desity (SSiClBD), SSiClBD + Field Capacity (SSiClBDFC) were used into ROSETTA subroutine program of RETC hierarchically to estimate van Geuchten water retention

parameters (α (cm⁻¹) and **n**). In addition to these estimations, van Genuchten's parameters were also obtained experimentally by using water retention data into inverse function of RETC computer program. New regression equations developed to estimate (α (cm⁻¹) and **n**) parameters for calibration of RETC estimated α and **n** parameters by using inverse function and basic soil parameters.

Statistical Analysis

Input parameters and estimated parameters were analyzed statistically using SPSS v13 program. Accuracy of estimations were evaluated using Corelation Coefficient (R) and Root Mean Squared Error (RMSE), expressed as,

$$RMSE = \left[\frac{1}{N}\sum_{i=1}^{N} (y_i - y_i)^2\right]^{1/2}$$
(4)

Where y_i refers the measured value, y_i is the predicted value, and *N* is the total number of observations. Negative and positive values of MR indicate under and over estimation. In addition **a** and **n** parameters, estimated by ROSETTA from basic soil parameters and estimated by inverse function of RETC using measured retention curve data, were regressed.

RESULTS and DISCUSSION

Summary statistics of input parameters (Table 1), and α and **n** parameters (Table 2) showed that among the input parameters clay (Cl), and among the α and **n** parameters estimated by ROSETTA α -SSiClBDFC and n-SSiCl parameters have the greatest C.V. values.

Table 1. Summary statistics of some soil physical properties used as inputs in ROSETTA to estimate van Genuchten water retention parameters

| | Minimum | Maximum | Mean | ¹ SD | 2 C.V. (%) |
|---|---------|---------|-------|-----------------|-----------------|
| 3 BD (gr cm ⁻³) | 1.13 | 1.78 | 1.45 | 0.13 | 1.15 |
| ⁴ FC (%) | 21.43 | 46.98 | 30.60 | 4.46 | 64.99 |
| ⁵ Ks (cm gün ⁻¹) | 41.60 | 154.74 | 93.07 | 24.03 | 620.55 |
| Clay(%) | 15.16 | 50.21 | 33.18 | 9.25 | 258.07 |
| Silt (%) | 23.44 | 42.50 | 31.81 | 3.63 | 41.50 |
| Sand (%) | 20.00 | 57.50 | 35.01 | 8.22 | 193.14 |

¹: SD, standard deviation, ²: CV, coefficient of variation, ³: BD, bulk density, ⁴: FC, filed capacity,

⁵: Ks, saturated hydraulic conductivity

| | Minimum | Maximum | Mean | ¹ SD | 2 C.V. (%) |
|---------------------------------|----------|---------|-------|-----------------|-----------------|
| α - ³ SSiCl | 8.40E-03 | 0.02 | 0.015 | 2.47E-03 | 0.04 |
| α - ⁴ SSiClBD | 7.40E-03 | 0.02 | 0.01 | 2.45E-03 | 0.04 |
| α - ⁵ SSiClBDFC | 3.70E-03 | 0.03 | 0.02 | 4.68E-03 | 0.13 |
| α - ⁶ Inverse | 6.27E-03 | 0.04 | 0.02 | 5.61E-03 | 0.20 |
| n- SSiCl | 1.27 | 1.52 | 1.37 | 0.06 | 0.26 |
| n- SSiClBD | 1.30 | 1.58 | 1.42 | 0.06 | 0.22 |
| n- SSiClBDFC | 1.25 | 1.53 | 1.35 | 0.05 | 0.22 |
| n- Inverse | 1.17 | 1.47 | 1.29 | 0.06 | 0.24 |

Table 2 Summary statistics of α and n parameters estimated by ROSETTA and obtained by inverse function of RETC computer model

¹: SD, standart deviation, ²: CV, coefficient of variation, ³: SSiCl; sand, silt and clay, ⁴: SSiClBD; SSiCl+Bulk Density (BD), ⁵: SSiClBDFC; SSiClBD+Field capacity (FC), ⁶: INVERSE, inverse function

Goodness-of-fit of α and n parameters estimated from basic soil parameters using ROSETTA were evaluated (Table 3). ROSETTA showed better performance to predict **n** parameter than α parameter. This is because fitting α parameter to air entry point is difficult than fitting the slope parameter **n** to retention curve.

| | ¹ R | ² RMSE |
|-------------------------------|----------------|-------------------|
| α - ³ SSiCl | 0.26 | 0.0055 |
| α - ⁴ SSiClBD | 0.30 | 0.0056 |
| α - ⁵ SSiClBDFC | 0.39 | 0.0059 |
| n - SSiCl | 0.69 | 0.0900 |
| n - SSiClBD | 0.53 | 0.1328 |
| n - SSiClBDFC | 0.61 | 0.0770 |

Table 3. Goodness-of-fit of the ROSETTA program in predicting α and n parameters from basic soil properties

¹: correlation coefficient, ²: RMSE, root mean square error; ³: SSiCl; sand, silt and clay, ⁴: SSiClBD; SSiCl+Bulk Density (BD), ⁵: SSiClBDFC; SSiClBD+Field capacity (FC)

Tomasella et al. (2000) stated these poor fits of retention points near saturation (Tomasella et al., 2000). Pachepsky and Rawls (2003) found that there is an important difference between the field and laboratory measured volumetric water contents for coarse, intermediate, and fine textured soils. As a result, poor prediction of the parameters might be due to measurement errors. Increase in the number of input variables such as organic carbon, and water contents at one or two potentials can improve the accuracy of soil hydraulic models (Schaap et al., 1998; Schaap and Leij, 1998; Minasny et al., 1999).

In addition to α and **n** parameters of ROSETTA, all input parameters of 100 soil sample are regressed with α -inverse and **n**-inverse to obtain best regression model of α and n (Eq. 5 and 6) to calibrate model for the filed studied. These regression models expressed as;

$$\alpha = 0.0086 - 0.00036 * FC + 0.000508 * clay$$
 (P<0.001, R2=0.54) (5)

$$n = 1.408 + 0.004 * FC - 0.007 * clay$$
 (P<0.001, R2=0.55) (6)

Goodness-of-fit of α and \mathbf{n} parameters obtained using developed regressions were given in Table 4. Compared to ROSETTA subroutine of RETC program estimations, Regression model estimations were better, increasing R for α from 0.39 to 0,736 and for n from 0.69 to 0.831.

Table 4. Goodness-of-fit of α and \mathbf{n} parameters obtained by regressing α -inverse and n-inverse parameters with basic soil properties

| | ^{1}R | ² RMSE |
|---|---------|-------------------|
| α | 0.736 | 0.0032 |
| n | 0.831 | 0.0331 |

¹: correlation coefficient, ²: RMSE, root mean square error

The other 68 soil data set were used for validation. Validity of regression model tested using 68 input data used in equation 5 and 6. Estimation results of regression models (α' and n') were correlated to measured data set (α -inverse and n-inverse), and results were given in Table 5. The results showed that R values found for validation data set were greatest as much as were for the regression data set

Table 5. Correlation of α' and n' parameters, obtained using validation data set into regression equations (6) and (7), with α -inverse and n-inverse parameters of validation data set

| α' | -0.988** | | |
|-------------------|----------|----------|-------------------|
| α -inverse | -0.703** | 0.716** | |
| n -inverse | 0.744** | -0.745** | -0.782** |
| | n' | lpha' | α -inverse |

^{*} Correlation is significant at the 0.001 level.

Minasny et al. (1999) implied that there was no linear relationship between the retention curve parameters and soil properties. That's why using linear regression for prediction of these parameters is not suitable. Further more, α and n curve shape parameters are quite sensitive to variability of soil properties as in this alluvial soil. The low performance of models to estimate α and n parameters might be due to the wide spatial and temporal variability in physical and hydraulic properties of alluvial soils.

CONCLUSIONS

In this paper, calibration of van Genuchten parameters using ROSETTA computer program and developed by regression analysis was presented. General performance of estimation ROSETTA is low for α , and is much better for **n**. Regression model for α and **n** developed using soil parameters of FC and clay content increased the estimation performance by increasing R value and decreasing RMSE values. Although prediction errors of ROSETTA are large, the results may be acceptable for most applications to predict soil hydraulic properties especially where hydraulic parameters are not available, and time, labor and money are limited.

REFERENCES

Blake, G.R, Hardge, K.H., 1986. Methods of Soil Analysis. Bulk Density, Part1.

- 2nd Ed. Agronomy 9. ASA and SSSA, 363-375, Madison.
- Gee, G.W., Bouder, J.W. 1986. Methods of Soil Analysis. Particle Size Analysis.
- Part 1. 2nd Ed. Agronomy 9. Am. Soc. Agron., 825-844, Madison
- Harter, T., Yeh, T.C.J., 1998. Flow in usaturated random porous media, nonlinear numerical analysis and comparison to analytical stochastic models. Advences in Water Resources. 22: 257-272.
- Kosugi, K., Hopmans, J.W., Dane, J.H., 1997. Water retention and storage: Parametric models. p. 739-757. In: J.H. Dane and G.C. Topp (ed.). Methods of soil analysis: Part 4- Physical methods.SSSA Book Ser. No. 5. SSSA, Madison, WI.
- Klute, A. 1986. Water Retention: Laboratory Methods. Methods of Soil Analysis.
- Part1. 2nd Ed. Agronomy 9. Am. Soc. Agron. 635-660, Madison.
- Klute, A., and Dirksen, C. 1986. Hydraulic conductivity and diffusivity:
- Laboratory methods. p. 687–734. *In* A. Klute (ed.) Methods of soil analysis. Part 1. 2nd. ed. Agron. Monogr. 9. ASA and SSSA, Madison, WI.
- Minasny, B., McBratney, A.B., Bristow, K.L., 1999. Comparison of different approaches to the development of pedotransfer functions for water-retention curves. Geoderma 93, 225–253.
- Muallem, Y., 1976. A new model for predicting the hydraulic conductivity of unsaturated porous media. Water Resources Research 12(3), 513-522.
- Pachepsky, Y.A., Rawls, W.J., 2003. Soil structure and pedotransfer functions. Eur. J. Soil Sci. 54, 443–451.
- Schaap, M.G., Leij, F.J., 1998. Using neural networks to predict soil water retention and soil hydraulic conductivity. Soil and Tillage Research. 47: 37-42
- Schaap, M.G., Leij, F.J., van Genuchten, M. Th., 1998. Neural network analysis for hierarchical prediction of soil water retention and saturated hydraulic conductivity. Soil Sci. Soc. Am. J. 62, 847-855.

- Schaap, M.G., Leij, F.J., 2000. Improved prediction of unsaturated hydraulic conductivity within the Muallem-van Genuchten model. Soil Sci. Soc. Am. J. 64, 843-851.
- Tartakovsky, D.M., Lu, Z., Guadagnino, A., 2003. Unsaturated flow in heterogeneous soils with spatially distributed uncertain hydraulic parameters. Journal of Hydrology. 275: 182-193
- Thomasson, M. J., Wierenga, P. J., 2003. Spatial Variability of the Effective Retardation Factor in an Unsaturated Field soils. Journal of Hydrology. 372:213-225
- Tomasella, J., Hodnett, M.G., Rossato, L., 2000. Pedo-Transfer Functions for the estimation of soil water retention in Brazilian soils. Soil Sci. Soc. Am. J. 64, 327 338.
- Tuli, A., Kosugi, K., Hopmans, J.W., 2001. Simultaneous scaling of soil water retention and unsaturated hydraulic conductivity functions assuming lognormal pore-size distribution. Advences in Water Resources. 24: 677-688
- van Genuchten, M. Th., 1980. A colsed-form equation for predicting the hydraulic conductivity of unsaturated soils. Soil Sci. Am. J. 44, 892-898.