

Determination of Unsaturated Hydraulic Conductivity in Field Conditions through Inverse Modelling Using Hydrus-1D

[¹] M. R. Namitha, [²] V. Ravikumar

[¹] Post Graduate student, Department of Soil and Water Conservation and Agricultural Structures,
 Tamil Nadu Agricultural University

[²] Professor and Head, Department of Soil and Water Conservation and Agricultural Structures,
 Tamil Nadu Agricultural University

Abstract: In this study, the unsaturated hydraulic conductivity (K) of sandy loam soil was determined through inverse modelling. The transient unsaturated water flow was simulated by numerically solving the Richards equation with the finite element code of Hydrus-1D. The cumulative infiltration flux across a boundary at different time was used as the input variable to optimise the soil hydraulic parameters. The inverse method generally uses a weighted least-squares approach in which numerically simulated data are fitted to the measured data. van Genuchten hydraulic model was chosen for the determination of unsaturated hydraulic conductivity. The soil hydraulic parameters viz. residual water content (θ_r), saturated water content (θ_s), inverse of air entry value (α), water retention parameter (n), and saturated hydraulic conductivity (K_s) were optimised in successive iterations. The optimised parameter values were fitted in the van Genuchten model for obtaining the unsaturated hydraulic conductivity of the proposed soil.

Keywords: Hydrus-1D, Inverse modelling, Unsaturated hydraulic conductivity

I. INTRODUCTION

Movement of water in soil is one of the important processes that influence the quality of soil and water in the environment. Soil water movement occurs under saturated as well as unsaturated conditions. Under saturated conditions the water flow is predominantly in horizontal direction which occurs below the water table, whereas under unsaturated conditions water flow is in vertical direction which occurs above the water table. The unsaturated zone plays an extremely important hydrologic role that influences water quality and quantity, ecosystem function and health, the connection between atmospheric and terrestrial processes, nutrient cycling, soil development, and natural hazards such as flooding and landslides. So, the knowledge of the hydraulic properties of unsaturated soils is essential for all studies involving water flow and solute transport in the vadose zone (Bitterlich et al., 2004). Simunek and van Genuchten (1996) estimated the unsaturated soil hydraulic properties from tension disc infiltrometer data by numerical inversion. Kodesova et al., (2003) determined the hydraulic properties of unsaturated soil using modified cone penetrometer by inverse modelling. Simunek et al., (1999) used the Hydrus-1D and Hydrus-2D codes for estimating unsaturated soil hydraulic and solute transport parameters. They used a parameter estimation procedure which combines the Levenberg-Marquardt nonlinear parameter optimization method involving weighted least squares with

either a one-dimensional numerical model (Hydrus-1D) or a two- or quasi three dimensional model (Hydrus-2D), which solve the governing equations for water flow and solute transport in variably-saturated porous media.

II. MATERIALS AND METHODS

Field Experiment

A double ring infiltrometer test was conducted in the field. The infiltration of water into the soil for different time periods were noted and the cumulative infiltration versus time graph (Fig.1) was plotted to analyse the trend of infiltration with respect to time.

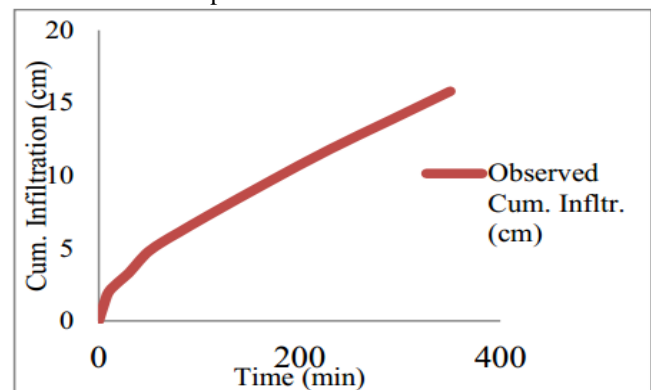


Fig. 1: Cumulative Infiltration vs. Time Curve for experimental data

Infiltration rate (i) is highest when water first enters the soil, and gradually decreases with time until a constant final rate is attained. This behaviour is also reflected in the cumulative infiltration (I) showing a rapid increase in infiltration at short times, which decreases gradually to a nearly linear rate of cumulative infiltration at large times.

Determination of Soil Physical Properties

Textural analysis of the soil was carried out to find the percentage of sand, silt and clay in the soil. After computing the relative percentage of different size groups, the triangular textural diagram can be used to find out the textural class of the soil. The percentage of sand, silt and clay obtained for the field soil were 72.5, 16.5 and 11% respectively. The soil comes under sandy loam category of textural class. The bulk density of the soil was calculated using core cutter method. In present study, the average bulk density of the proposed sandy loam soil was found to be 1.58 g cm⁻³. Variably Saturated Flow Equation (Richard's Equation) The transient flow through unsaturated zone was simulated using the numerical model proposed by Richard (1931):

$$\frac{\partial \theta(h)}{\partial t} = \frac{\partial(K(h) \frac{\partial h}{\partial z})}{\partial z} + \frac{\partial K(h)}{\partial z} - S(h) \quad (1)$$

where, θ is the soil moisture content, $K(h)$ is the unsaturated hydraulic conductivity function, $S(h)$ is the sink term, h is the pressure head and t is the time. This partial differential equation is the equation governing variably saturated flow in unsaturated zone. Eq. (1) is the mixed form of the Richard's equation having two dependent variables: θ and h .

Soil Hydraulic Properties Function

A model of the unsaturated soil hydraulic properties must be selected prior to application of the numerical solution of the Richard's equation. This study used the unsaturated soil hydraulic functions of van Genuchten (1980). These functions are given by: Effective Saturation,

$$S_e = \frac{1}{[1+(-\alpha h)^n]^m} \quad (2)$$

and, $m = 1 - \frac{1}{n}$

where, h is the pressure head (cm) and, S_e is the effective saturation (-).

$$S_e = \frac{\theta_h - \theta_r}{\theta_s - \theta_r} \quad (3)$$

where, θ_h is the volumetric moisture content (cm³cm⁻³).

The volumetric moisture content of the soil,

$$\theta_h = \theta_g * \text{Specific gravity} \quad (4)$$

where, θ_g is the gravimetric moisture content (cm³cm⁻³).

$$\text{Specific gravity} = \frac{\text{Dry Density of soil}}{\text{Density of water}} \quad (5)$$

The density of the water is 1 g cm⁻³ and the dry density of soil was calculated as 1.58 g cm⁻³ using core cutter method.

Unsaturated hydraulic conductivity,

$$K = K_s S_e^l [1 - (1 - S_e^m)^n] \quad (6)$$

where, θ_r is the residual volumetric water content, [L³ L⁻³], θ_s is the saturated volumetric water content, [L³ L⁻³], S_e is the effective saturation [-], h is the soil water matric head [L], K_s is the saturated hydraulic conductivity [L T⁻¹], l is the pore connectivity coefficient [-], α [L⁻¹] and $m = 1 - 1/n$ are empirical coefficients. The pore-connectivity parameter l in the hydraulic conductivity function was estimated by Mualem (1976a) to be 0.5 as an average for many soils.

Inverse Modelling

The solution of an inverse problem entails determining unknown causes by numerical modelling approach, based on observation of their effects. The inverse method includes three interrelated functional parts (i) a controlled transient flow experiment for which boundary and initial conditions are prescribed and various flow variables are measured, such as cumulative infiltration and/or drainage cumulative and/or matric head and/or water content; (ii) a numerical flow model simulating the transient flow regime of this experiment, using initial estimates of the parametric soil hydraulic functions; and (iii) an optimization algorithm, which estimates the unknown parameters through minimization of the difference between observed and simulated flow variables (residuals) defined in an objective function () through an iterative solution of the transient flow equation. Desired hydraulic parameters are determined by systematically minimizing the differences between observed and simulated state variables. The total of these differences is expressed by an objective function, which may be defined as:

$$\Phi(\beta, y) = \sum_{j=1}^{j=m_y} v_j \sum_{i=1}^{i=n_j} w_{ij} [y_j^*(z, t_i) -$$

$$y_j(z, t_i, \beta)]^2 \quad (7)$$

where, the right-hand side represents the residuals between the measured (y_j^*) and corresponding model-predicted (y_j) space-time variables using the soil hydraulic parameters of the optimized parameter vector, . The first summation sign

sums the residual for all measurement type, whereas the variable in the second summation denotes the number of measurements for a certain measurement type j . Typically, in water flow studies, may represent water flux density, cumulative water flow, soil water matric head, or soil water content values. Weighting factor values for can be selected such that data types are weighted equally using a normalization procedure or such that they are equal to the reciprocal of the variance of measurement type j ; additional weighting can be assigned to individual data (Hollenbeck *et al.*, 2000). *Parameter Optimization through Inverse Modelling* The Hydrus-1D numerical model which uses the one-dimensional Richard's transient flow equation has an inverse modelling capability. An objective function, which includes deviations between measured and predicted variables such as pressure heads or water contents at different depths and times, is minimised. Minimization of the objective function is accomplished using the Marquardt-Levenberg nonlinear minimization (Marquardt 1963). In present study, the cumulative infiltration flux across a boundary at different time was used as the input variable to optimise the soil hydraulic parameters through inverse modelling. Hydrus-1D has the provision for selecting an appropriate model for simulation of the available data. In this study, the van Genuchten model was chosen for simulating the transient water flow in the soil. The model optimises six soil hydraulic parameters viz. residual water content (θ_r), saturated water content (θ_s), inverse of air entry value (α), pore connectivity parameter (l), water retention parameter (n) and saturated hydraulic conductivity (K_s), which are necessary to calculate the unsaturated hydraulic conductivity. The initial estimates for the parameters were estimated from Rosetta Lite v.1.1 module incorporated with Hydrus-1D. The initial estimates were predicted by the model from the basic soil data including the percentage sand, silt, clay and the bulk density of the soil.

Table 1: Initial Parameter Estimates as per Rosetta Lite v. 1.1

Parameters	Initial Estimates (as per Rosetta Lite v. 1.1)
Residual soil water content, θ_r ($\text{cm}^3\text{cm}^{-3}$)	0.0450
Saturated soil water content, θ_s ($\text{cm}^3\text{cm}^{-3}$)	0.3684
Inverse of the air-entry value (or bubbling pressure), α (cm^{-1})	0.0356
Parameter n in the soil water retention function	1.4884
Saturated hydraulic conductivity, K_s (cm min^{-1})	0.0289
Pore-connectivity parameter, l (-)	0.5000

The user can specify the type of upper and lower boundary conditions to be used. In the present study, since the ponding depth in the ring varied with time, a Variable Pressure Head upper boundary condition was given and the lower boundary condition was selected as Free Drainage. The initial condition can be specified either in terms of the pressure head or the water content. In this study, the initial pressure head at the soil surface and at 75 cm depth were calculated using Eq. (2) and Eq. (3). So, the initial conditions were specified in terms of pressure head. In this study, the pressure head at the top boundary varied with respect to time. At the start of the experiment, a 10 cm depth of water is maintained in the double ring infiltrometer (i.e. $h_{Top} = 10\text{cm}$ at 0.01minutes). As time passes, water got infiltrated into the soil and the ponding height was decreased. After 5 minutes the water level decreased to 8.9 cm (i.e. $h_{Top} = 8.9$ cm at 5 minutes), which shows that 1.1 cm water got infiltrated into the soil in 5 minutes. At each time after the reading was taken, the water was refilled to 10 cm (i.e. $h_{Top} = 10$ cm at 5.01 minutes). Likewise, the time dependent boundary conditions for 350 minutes were entered. The initial pressure head at the top (i. e. soil surface) and the bottom (i. e. 75 cm below the soil surface) of the soil profile were determined using the expressions for hydraulic functions (Eq. (2) and Eq. (3)) by van Genuchten (1980). The values of the hydraulic parameters viz. , n and α were taken from the initial parameter estimates. The pressure heads at top and bottom were calculated as -1250 cm and -300 cm respectively. Since no further reduction in the Sum of Squares (SSQ) was obtained, the optimisation of the objective function had stopped with 12 iterations.

III. RESULTS AND DISCUSSIONS

Inverse methods are increasingly used to estimate the hydraulic properties of unsaturated soils nowadays. In this study, the Hydrus-1D numerical code which uses the one dimensional Richard's equation was used for the numerical inversion of six soil hydraulic parameters including saturated water content (θ^s), residual water content (θ^r), saturated hydraulic conductivity (K_s) soil water retention parameter (n), inverse of air entry value (α) and pore connectivity parameter (l). Hydrus-1D allows the optimization of these parameters using Marquardt-Levenberg optimization algorithm. The optimised parameters were fitted to the empirical models proposed by van Genuchten (1980) for finding the unsaturated hydraulic conductivity (K) and the water retention properties of the proposed sandy loam soil. Comparison of Observed and Simulated Data Once the optimization was completed successfully, Hydrus generated a set of simulated data for

the observed cumulative infiltration data. The comparison of observed and simulated data is generally termed as Residual Analysis. After evaluation of the uniqueness of an inverse solution, the next logical step is to compare the simulated results with the corresponding field observations. Table 2 shows the field observed data and corresponding simulated data obtained for different time steps.

Table 2: Measured cumulative infiltration from field and fitted data using Hydrus-1D

S. No.	Time (min)	Observed Cumulative Infiltration (cm)	Simulated Cumulative Infiltration (cm)
1	0	0.00	0.00
2	5	-1.10	-1.38
3	10	-2.00	-1.94
4	20	-2.70	-2.78
5	30	-3.30	-3.46
6	40	-4.10	-4.06
7	50	-4.80	-4.61
8	65	-5.50	-5.37
9	80	-6.10	-6.08
10	110	-7.30	-7.37
11	170	-9.60	-9.65
12	230	-11.80	-11.77
13	290	-13.80	-13.82
14	350	-15.80	-15.80

*Hydrus considers the infiltration data as negative flux

Analysis of the table values (Table 2) shows a best fit between the observed and simulated cumulative infiltration data. For example, after 5 min of the experiment, the observed cumulative infiltration was 1.10 cm; the data simulated by Hydrus at 5 min was 1.38 cm which was almost similar to the observed data. Similarly, at 230 min, the observed and fitted data were 11.80 and 11.77 cm respectively. The table shows a significant correspondence between the observed and the fitted data. Infiltration data was generated to analyse the accuracy of flow predictions by Hydrus-1D. Fig. 2 shows the measured and calculated cumulative infiltration curves when the objective function was defined in terms of the cumulative infiltration data. Results indicate excellent agreement between the measured and optimized infiltration curves.

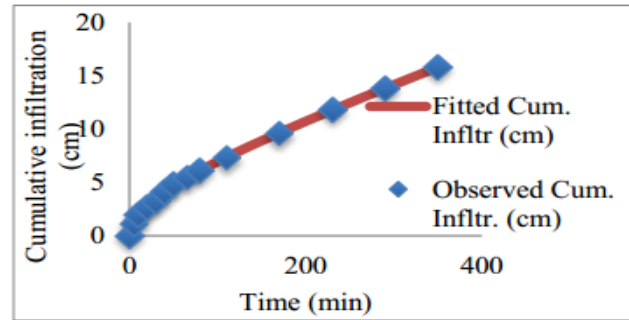


Fig. 2: Measured cumulative infiltration from field (data points) and fitted cumulative infiltration using Hydrus-1D

The plot of observed and fitted cumulative Final parameter estimates The van-Genuchten Maulem soil hydraulic parameters were optimized using the objective function defined in terms of the measured variable, i.e., cumulative infiltration depths. The Hydrus numerical code optimised the initial estimated parameters in consecutive iterations to get an optimum parameter set. In this study, the solution got converged in 12 consecutive iterations. The sum of squares (SSQ) was reduced to the minimum with 12 iterations. Since no further reduction in SSQ was possible, the iterations were stopped and final outputs were obtained. The lists of initial and final estimates of the six optimized parameters are shown in the Table 3. There is a good correspondence between the initial and optimised parameter estimates of θ_r , θ_s , α , n and K_s . In most of the studies, the pore connectivity parameter (l) is fixed as a constant value of 0.5 which is an average value for all types of soils. But in present study, l has been optimized to get a better value for the unsaturated hydraulic properties for the proposed sandy loam soil. The initial and final estimates of l show significant difference in this study. The optimized parameter values for α , n and K_s were mostly very close or only slightly different than the initial parameter values. The close correspondence of the initial and final estimates of K_s lends further credibility to the accuracy of double ring infiltrometer data, for the sandy loam soil used in this study

Table 3: Initial and Final estimates for six parameters

Parameters	Initial Estimates	Final Estimates
θ_r ($\text{cm}^3 \text{cm}^{-3}$)	0.0450	0.0445
θ_s ($\text{cm}^3 \text{cm}^{-3}$)	0.3684	0.3719
α (cm^{-1})	0.0356	0.0251
n	1.4884	1.5181
K_s (cm min^{-1})	0.0289	0.0279
l	0.5000	0.0003

A reasonably good description of the hydraulic data was obtained when setting the pore connectivity factor to 0.5 because l was not sensitive to the fitting data (Wessolek et al, 1994). A wide range of values has been reported for l . For example, Schuh and Cline (1990) found values ranging from -8.73 to 14.80, while Wosten and van Genuchten (1988) reported values between -16 and 2.2 for medium- and fine-textured soils. From these and other studies (e.g. Yates et al., 1992), it appears that the value of l has only a relatively small effect on the objective function, (Φ) . Therefore, as suggested by Mualem (1976a), l was fixed at 0.5 for the second simulation.

Table 4: Initial and Final Parameter estimates with l fixed as 0.5

Parameters	Initial Estimates	Final Estimates
θ_r ($\text{cm}^3 \text{cm}^{-3}$)	0.0450	0.0650
θ_s ($\text{cm}^3 \text{cm}^{-3}$)	0.3684	0.3362
α (cm^{-1})	0.0356	0.0321
n	1.4884	1.8416
K_s (cm min^{-1})	0.0289	0.0271

Correlation matrix

Table 3 shows the optimised parameters with l fixed as 0.5, an average value for all soils. The results reveal that all the parameters exhibit a slightly noticeable change from the initial estimates when the pore connectivity parameter was fixed as 0.5. As part of the inverse solution, Hydrus produces a correlation matrix, which specifies degree of correlation between the fitted coefficients. The correlation matrix quantifies changes in model predictions caused by small changes in the final estimate of particular parameters. The correlation matrix reflects the non orthogonality between two parameter values. A value of ± 1 suggests a perfect linear correlation whereas 0 indicates no correlation at all. 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 (Radcliff and Simunek, 2010). High correlation causes underestimation of parameter uncertainty, slows down convergence rate, and increases non-uniqueness.

Table 5: Correlation table for optimized parameters

	θ_r	θ_s	α	n	K_s	l
θ_r	1					
θ_s	-0.78	1				
α	-0.53	0.88	1			
n	0.89	-0.81	-0.45	1		
K_s	0.59	-0.89	-0.99	0.48	1	
l	0.13	-0.45	-0.29	0.43	0.23	1

Soil Water Retention Curve Table 5 shows the correlation table for the optimised parameters in present study. The correlation table shows a large correlation (0.8997) between n and θ_r for the infiltration experiment, a result that is common when fitting retention data to the van Genuchten relationship. A highest negative correlation is observed between α and K_s . This means that even a slight change in α value can lead to corresponding change in the saturated hydraulic conductivity K_s . The relation between pressure head and volumetric water content in a soil is termed the soil water retention curve or soil moisture characteristic curve. The differences between soil water retention curves are attributed primarily to the differences in pore size distribution among soils. These curves are sensitive to changes in bulk densities and the disturbance of soil structures.

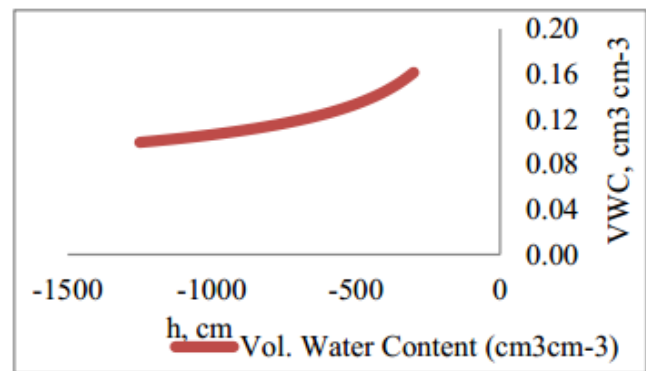


Fig. 3: Soil Water Retention Curve

Fitting the simulated data of volumetric soil water content (θ_h) and pressure head (h) to the model described by van Genuchten (1980) gives the regression curve (water retention curve) which is illustrated in Fig. 3.

Unsaturated Hydraulic Conductivity vs. Pressure Head Curve

At very low water contents, continuous fluid paths may not exist and water may move in vapour phase. The unsaturated hydraulic conductivity is therefore represented as a function of negative pressure head ($K(h)$) or as a function of water content ($K(\theta)$). Substitution of parameters n and m ($= 1 - 1/n$) into the equation for unsaturated hydraulic conductivity function and plotting the unsaturated hydraulic conductivity versus pressure head gives the Fig. 4, which is the graphical representation of Mualem's model (1976). In the unsaturated zone, larger pores drain more readily than smaller ones. Therefore, the hydraulic conductivity is much less under unsaturated than saturated conditions because of water moving through smaller pores or as films along the walls of larger pores. The average saturated hydraulic conductivity for the sandy loam soil under study was found

as 0.027 cm min⁻¹ (38.88 cm d⁻¹) through inverse modelling using Hydrus-1D. From Fig. 4, the unsaturated hydraulic conductivity was found to be in the range of near zero to 0.07 cm d⁻¹, which is much lesser than the saturated hydraulic conductivity.

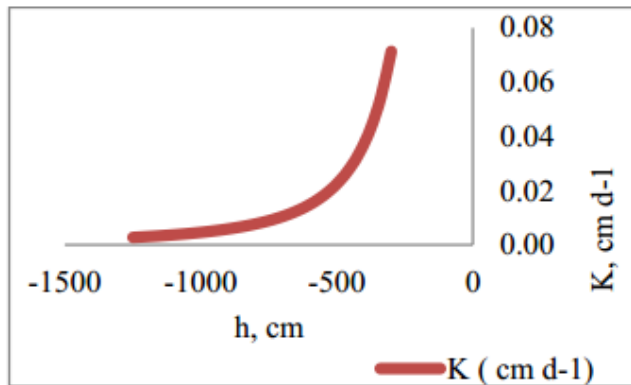


Fig. 4: Unsaturated hydraulic conductivity vs. pressure head curve

The unsaturated hydraulic conductivity increases with decrease in the negative pressure head. A rapid increase in the K value is observed when the negative pressure head decreases beyond 500 cm.

Unsaturated Hydraulic Conductivity vs. Moisture Content Curve

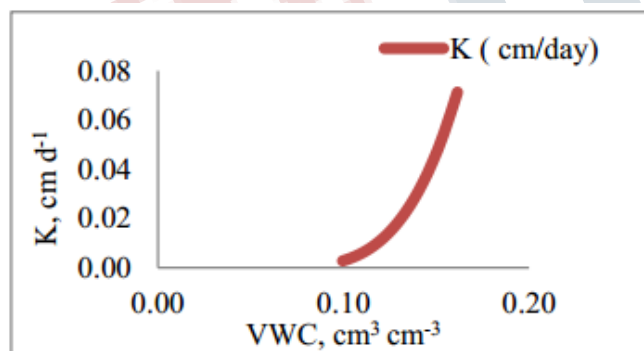


Fig. 5: Unsaturated hydraulic conductivity vs. Volumetric Water Content

The relationship between the volumetric soil water content and the unsaturated hydraulic conductivity was well shown in Fig. 5. The volumetric water content and the unsaturated hydraulic conductivity show a direct relationship with each other. Summary and Conclusion The movement of water in the unsaturated zone is an important process to be considered. In this study, the Hydrus numerical model was effectively utilised for the optimisation of six soil hydraulic parameters including θ_r , θ_s , α , n , K_s and l using inverse modelling. There was a good correspondence between the

initial and final parameter estimates. The observed and simulated cumulative infiltration data also revealed a best fit. The optimised parameter values were substituted in the van Genuchten model and found the unsaturated hydraulic conductivity and water retention properties of the sandy loam soil under study.

REFERENCES

1. Bitterlich, S., W. Durner, S. C. Iden, and P. Knabner. 2004. Inverse estimation of the unsaturated soil hydraulic properties from column outflow experiments using freeform parameterizations. *Vadose Zone Journal* 3: 971–981.
2. Hollenbeck, K.J., J. Simunek, and M. Th. Van Genuchten. 2000. RETCML: Incorporating maximum-likelihood estimation principles in the soil hydraulic parameter estimation code RETC. *Comput. Geosci.* 26:319–327.
3. Kodesova, R. 2003. Determination of hydraulic properties of unsaturated soil via inverse modelling. Lecture given at the College on Soil Physics, Trieste, 3-21 March: 223- 230.
4. Marquardt, D. W. 1963. An algorithm for leastsquares estimation of nonlinear parameters. *Journal of the Society for Industrial and Applied Mathematics.* 11(2):431-441.
5. Maulem, Y. 1976a. A new model for predicting the hydraulic conductivity of unsaturated porous media. *Water Resour. Res.* 12: 513-522.
6. Radcliff, D. E., and J. Simunek. 2010. *Soil Physics with Hydrus: Modeling and Applications* CRC Press: 183-347.
7. Richards, L.A. 1931. Capillary conduction of liquids through porous mediums. *Physics* 1:318–333.
8. Schuh, W.M. and R. L. Cline, 1990. Effect of soil properties on unsaturated hydraulic conductivity pore-interaction factors. *Soil Sci. Soc. Am. J.* 54: 1509-1519.
9. Simunek, J., and M. Th. van Genuchten. 1996. Estimating unsaturated soil hydraulic properties

from tension disc infiltrometer data by numerical inversion. *Water Resour. Res.* 32(9): 2683–2696.

10. Simunek, J., O. Wendroth, and M. Th. Van Genuchten. 1999. Estimating unsaturated soil hydraulic properties from laboratory tension disc infiltrometer experiments. *Water Resour. Res.* 35(10): 2965–2979.
11. van Genuchten, M. Th. 1980. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. *Soil Sci. Soc. Am. J.* 44: 892–898.
12. Wessolek, G., R. Plagge, F. J. Leij, and M. Th. Van Genuchten. 1994. Analysing problems in describing field and laboratory measured soil hydraulic properties. *Geoderma* 64: 93-110.
13. Wosten, J. H. M., and M. Th. van Genuchten. 1988. Using texture and other soil properties to predict the unsaturated soil hydraulic functions. *Soil Sci. Soc. Am. J.* 52: 1762- 1770.
14. Yates, S. R., M.Th. van Genuchten, A. W. Warrick, and F. J. Leij. 1992. Analysis of measured, predicted and estimated hydraulic conductivity using the RETC computer program. *Soil Sci. Soc. Am. J.*, 56: 347-354