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Soil Hydraulic Parameters Estimation through Inverse Modeling from Double Ring Infiltrometer Data using HYDRUS-1D

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ABSTRACT

In this study, HYDRUS-1D was used to simulate the ponded infiltration through double ring infiltrometers into a hypothetical sandy loam soil. The soil hydraulic parameters were optimized by inverse modeling. The optimized soil hydraulic parameters were residual water content, (ϑ_r = 0.0076 cm^3 cm^{-3}), saturated water content, (ϑ_s = 0.3103 cm^3 cm^{-3}), inverse of the air entry value (α = 0.0011 cm^{-1}), parameter *n* in the soil water retention function (n=1.337), saturated hydraulic conductivity (K_s=0.0238 cm min^{-1}) and pore connectivity parameter, (*l*=0.0011) respectively. The average saturated hydraulic conductivity for the sandy loam soil under study was found as 0.0238 cm min^{-1} (34.27 cm day^{-1}) through inverse modeling. The unsaturated hydraulic conductivity was found to be in the range of 0 to 0.063 cm day^{-1}, which is much smaller than saturated hydraulic conductivity. The model performance was evaluated by the root mean square error, correlation coefficient and model efficiency and it was found that 0.003 cm, 0.99 and 0.99 respectively. From the results, it was concluded that the HYDRUS-1D model is a very good tool for simulating water flow as well as optimization of soil hydraulic parameters through an inverse solution.

Key words: HYDRUS, Inverse modeling, Infiltration, Soil hydraulic parameters, Hydraulic conductivity

The importance of the unsaturated zone as an integral part of the hydrological cycle has long been recognized. The vadose zone plays an important role in many aspects of hydrology, including infiltration, soil moisture storage, evaporation, plant water uptake, groundwater recharge, runoff, and erosion. Simultaneous movement of water and heat in the vadose zone of arid and/or semi-arid regions is of great interest in evaluating water and energy balance of subsurface environments in both agricultural and engineering applications (Nakhaei *et al.* 2014). Unsaturated water flows generally described by using the Richards equation. When the inverse modeling approach is used, the unknown hydraulic parameters are estimated by minimizing deviations between observed variables and model-predicted output for transient flow experiments.

Russo *et al.* (1991) analyzed the infiltration events in relation to soil hydraulic properties by inverse problem methodology. In which, the saturated conductivity (K_s), in the estimation criterion enhance the positive correlation and stability of the provided solution. Gribb (1996) did a numerical analysis with cone penetrometer experiment, including a study of identifiability of the soil hydraulic parameters. It was found that the saturated hydraulic conductivity (K_s) and the bubbling pressure (α) are most reactive and the saturated water content (θ_s) and the parameter (*n*) are least reactive in van Genuchten's (1980) retention function to the inverse solution. Šimůnek and Genuchten (1996) estimated the unsaturated soil hydraulic properties by numerical inversion method using data collected from tension disc infiltrometer. The adopted numerical inversion method is a parameter optimization procedure which combines the Levenberg-Marquardt nonlinear optimization method and quasi-three-dimensional numerical model.

I-Lopmans (1999) reviewed the studies on inverse estimation of soil hydraulic properties. As per the review, the benefits of inverse modeling are given as a) it mandates the combination of experimentation with numerical modeling, b) experiments are transient, providing fast results, c) inverse procedures yields the parameter of soil water retention and unsaturated hydraulic conductivity in a single experiment and d) the parameter optimization also provides a confidence interval of the optimized parameters. Šimunek *et al.* (2012) conducted a study on the use, calibration, and validation of Hydrus numerical model. The results imply that the Marquardt Levenberg approach was simple and gradient-based optimization for the estimation of hydraulic parameters. Mashayekhi *et al.* (2016) used Hydrus-2D/3D ponded infiltration through double-ring infiltrometers into a hypothetical loamy soil profile. Hydrus software package is used for creating double ring infiltrometer domain and the generation of infiltration data by a direct simulation method. The study used twelve scenarios of inverse modeling (divided into 3 groups) for the estimation of Maulem-van Genuchten hydraulic parameters. The results also inferred that the simulation error was reduced by reducing the hydraulic parameters in the optimization process. The main objective of this study was to optimize the soil hydraulic parameters by inverse modeling, estimation of unsaturated hydraulic conductivity and validated the HYDRUS-1D model by simulated cumulative infiltration data compared with observed cumulative infiltration.

MATERIALS AND METHODS

The double ring infiltrometer test was conducted in C3 block at the Central Farm of Agricultural Engineering College and Research Institute, Kumulur, Trichy District. The inner and outer ring radii were 15 and 30 cm, respectively, and the insertion depth of the rings was considered to be 7 cm. The depth of water maintained in inner and outer rings was 10 cm. The experiment was continued for 540 minutes. The observation was taken at a regular interval.

Determination of soil physical properties

Soil texture analysis and soil bulk density were done by International Robinson pipette method and core cutter method respectively.

Soil texture: Textural analysis of the soil was carried out to find the percentage of sand, silt, and clay in the soil. Soil samples were collected from different layers up to the depth of 60 cm. The soil collected from the study area was air dried for one day and it was then passed through 2 mm sieve. In the present study, the soil texture of three different soil layers at three locations in the field was found out and the average value of percentage sand, silt and clay were used for parameter optimization.

Bulk density

In the present study, the dry bulk density at three different soil layers for three random samples from the field was found out and the average dry bulk density was calculated.

HYDRUS-1D model

Water flow simulations were conducted with the Hydrus-1D model, which numerically solves the Richards equation (Radcliffe and Simunek 2010):

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(K\frac{\partial h}{\partial z} + K\right) \quad \ldots\ldots\ldots\ldots\ (1)$$

Where θ is the volumetric moisture content in [L^3L^{-3}]; t is time [T]; z is the vertical coordinate; h is pressure head [L]; K is the hydraulic conductivity [LT^{-1}];

Parameters of the soil hydraulic functions are updated iteratively in the optimization routine, thereby continuously reducing the residuals until a predetermined convergence criterion has been achieved. 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 ϕ, which may be defined as (Šimunek *et al.* 2012):

$$\phi(b,q) = \sum_{i=1}^{n_{qj}} w_{i,j}[q_j^*(x,t_j) - q_j(x,t_i,b)]^2 \quad \ldots\ldots\ldots\ (2)$$

Where the first term on the right side represents deviations between measured and calculated space-time variables. In this first term, n_{qj} is the number of measurements within a particular measurement set, $q^*_j\ (x,\ t_i)$ represents specific measurements at time t_i for the j_{th} measurement set at location x, $q^*_j\ (x,\ t_i,\ b)$ represents the corresponding model predictions for the vector of optimized parameter b, and $w_{i,j}$ are weights associated with a particular measurement set respectively.

Among the various nonlinear optimization techniques available for minimizing the objective function, the Marquardt-Levenberg–method is the most widely used. This method uses a weighted least-squares approach based on Marquardt's maximum neighborhood method. The complete procedure for parameter optimization by the HYDRUS-1D model was shown in (Table 1).

Table 1 Input parameters for parameter optimization

Model parameters	Name of the parameters	Value/type/unit
Main process	Water flow	
	Inverse solution	
Inverse solution	Soil hydraulic parameters	
	No internal weighting	
	Maximum no. of iterations	50
	No. of data points in the objective function	15
Geometry information	Type of geometry	1D- vertical plane
	Length units	cm
	No. of soil material	1
	No. of layers for mass balance	1
	The decline from vertical axes	1

	The depth of soil profile	60
Time information	Time units	Minutes
	Time discretization	
	Initial time	0
	Final time	540
	Initial time step	0.0001
	Minimum time step	0.000001
	Maximum time step	0.5
	No. of time variable boundary conditions	30
Print information	Number of print times	15
Soil hydraulic model	Hydraulic model	van Genucthen-Mualem
	Hysteresis	No hysteresis
Water flow parameters	No of material	1
Time variable boundary condition	Time	Minutes
	Variable pressure head	cm
Data for inverse solution	Time	Minutes
	Cumulative infiltration depth	cm
	Type	0
	Position	1
	Weight	1
Domain properties	Material distribution	1
	Sub-regions	1
Initial conditions	Pressure head	
	Top	-1683.5 cm
	Bottom	-396 cm
Boundary conditions	Surface boundary	Variable pressure head
	Bottom boundary	Free drainage

Soil hydraulic properties function

Soil hydraulic properties characterizing soil water retention and hydraulic conductivity were described using analytical functions of van Genuchten (1980). Soil hydraulic properties were estimated with van Genuchten function as follows ((Han *et al.* 2015):

$$\theta(h)=\begin{cases}\theta_r+\dfrac{\theta_s-\theta_r}{[1+(\alpha h)^n]^m};\ h<0\\ \theta_s;\ h\geq 0\end{cases} \quad \text{………… (3)}$$

$$S_e(h)=\frac{\theta(h)-\theta_r}{\theta_s-\theta_r}=\frac{1}{(1+|\alpha h|^n)^m} \quad \text{………… (4)}$$

Where $\theta(h)$ is the volumetric water content [L^3L^{-3}]

Combination of the above equation (2.3 and 2.4) with Mualem's (1976a) hydraulic conductivity model leads to the following expression for hydraulic conductivity given by Van Genuchten (1980) are:

$$K(\theta)=K_s\ S_e^l[1-\left(1-S_e^{\frac{1}{m}}\right)^m]^n \quad \text{………… (5)}$$

Where, S_e is the effective saturation [-]; θ is the volumetric moisture content in [L^3L^{-3}]; h is pressure head [L]; K_s is the saturated hydraulic conductivity [LT^{-1}]; θ_r is the residual volumetric water contents [L^3L^{-3}]; θ_s is the saturated volumetric water contents [L^3L^{-3}]; l is the pore connectivity coefficient [-]; α [L^{-1}] and m=1-1/n are empirical coefficients. The pore-connectivity parameter l in the average hydraulic conductivity function for many soils is 0.5 (Mualem 1976).

In order to validate the numerical simulation by HYDRUS-1D for soil hydraulic parameter optimization, observed and simulated cumulative infiltration data at 16 discretize times including 0, 5, 10, 20, 30, 45, 60, 90, 120, 180, 240, 300, 360, 420, 480 and 540 min were used for statistical comparisons. The model performance was evaluated by a root mean square error (RMSE) (Li *et al.* 2015), correlation coefficient (R^2) (Singh *et al.* 2013) and model efficiency (MF) (Singh *et al.* 2013):

$$RMSE=\frac{1}{n}[\sum_{i=1}^{n}(P_i-O_i)^2]^{1/2} \quad \text{………… (6)}$$

$$R^2=\frac{\left\{\sum_{i=1}^{n}(O_i-O)(P_i-P)\right\}^2}{\sum_{i=1}^{n}(O_i-O)^2\sum_{i=1}^{n}(P_i-P)^2} \quad \text{………… (7)}$$

$$MF=1-\frac{[\sum_{i=1}^{n}(P_i-O_i)^2]}{[\sum_{i=1}^{n}(O_i-O)^2]} \quad \text{………… (8)}$$

Where, P_i is the predicted value; O_i is the observed value; P is the mean predicted value; O is the mean observed value; n is the number of compared values.

RESULTS AND DISCUSSION

In the present study, the soil texture and bulk density of three different soil layers at three locations in the field was found out and the average value of percentage sand, silt and clay were used for parameter optimization. The determined soil texture and bulk density are shown in (Table 2).

Table 2 Physical properties of the soil of the experimental field

Depth (cm)	Mineral content (%)			Textural class	Bulk density (g cm^{-3})
	Sand	Silt	Clay		
0-20	72	14.6	13.4	Sandy Loam	1.58
20-40	70	16.6	13.4	Sandy Loam	1.33
40-60	76.6	12.5	10.9	Sandy Loam	1.33
Average	72.87	14.57	12.56	Sandy Loam	1.413

Infiltration characteristics and saturated hydraulic conductivity

From double ring infiltrometer, the infiltration rate and saturated hydraulic conductivity were found as 1.71 cm h^{-1} and 41.1 cm day^{-1}respectively. The soil hydraulic parameters were estimated by inverse modeling using obtained cumulative infiltration depth at a different time interval.

Parameter optimization through inverse modelling

Once the optimization was completed successfully, HYDRUS generates 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 by residual analysis, the next logical step is to compare the simulated results with the corresponding field observations. (Fig 1) shows the field observed data and corresponding simulated data obtained at different time steps. There exists a best fit between the observed and simulated infiltration depth.

Final parameter estimates

The van Genucthen-Mualem (VGM) soil hydraulic parameters were optimized using the objective function defined I term of the measured variable, i.e. cumulative infiltration depths. The HYDRUS numerical code optimized the initially estimated parameters in consecutive iterations to get an optimum parameter set in this study. The solution got converged in 34thconsecutive iterations. The sum of squares was reduced to the minimum with 34 iterations. (Table 3) shows the optimized parameters with *l* fixed as 0.5.

The parameter optimization was done for without fitting the pore connectivity parameter denoted as *l*. In most of the studies, pore connectivity parameter (*l*) is fixed as a constant which is an average value for all types of soils because *l* was not sensitive to the fitting data. The optimized parameters residual water content, θ_r and an inverse of the air entry value α slightly varied as compared to initial parameter values (Table 4).

Table 3 Initial and Final estimates with l fixed as 0.5 by using HYDRUS-1D

Parameters	Initial estimates	Final estimates
Residual water content, θ_r (cm^3 cm^{-3})	0.0518	0.0501
Saturated water content, θ_s (cm^3 cm^{-3})	0.4169	0.2910
An inverse of the air entry value α, (cm^{-1})	0.0300	0.0013
Parameter *n* in the soil water retention function	1.5281	1.3840
Saturated hydraulic conductivity $K_{s,}$ (cm min^{-1})	0.0511	0.0238

Table 4 Initial and Final estimates for six parameters by HYDRUS-1D

Parameters	Initial estimates	Final estimates
Residual water content, θ_r (cm^3 cm^{-3})	0.0518	0.0076
Saturated water content, θ_s (cm^3 cm^{-3})	0.4169	0.3103
An inverse of the air entry value α, (cm^{-1})	0.0300	0.0011
Parameter *n* in the soil water retention function	1.5281	1.3370
Saturated hydraulic conductivity $K_{s,}$ (cm min^{-1})	0.0511	0.0238
pore connectivity parameter *l*	0.5	0.0011

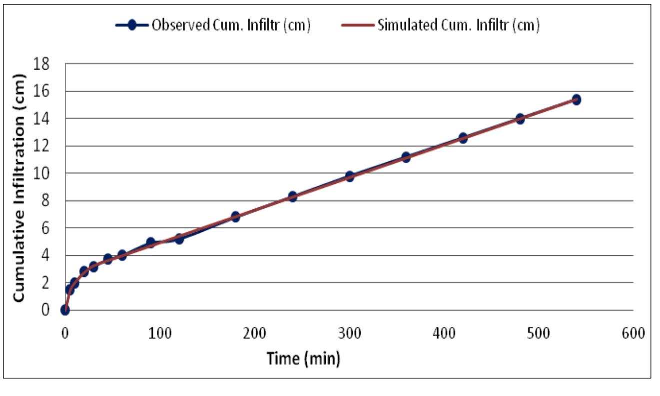

Fig 1 Observed cumulative infiltration from the field and simulated cumulative infiltration by HYDRUS-1D

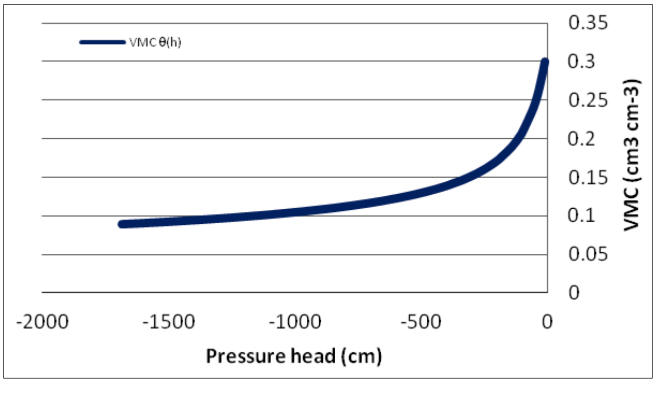

Fig 2 Obtained soil water characteristics curve by HYDRUS

Soil water characteristics 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 which is illustrated in (Fig 2). It was also observed that the soil matric suction was increased negatively with a decrease in volumetric water content. The volumetric water content at -10 and -1683 cm pressure head was obtained as 0.299 and 0.09 cm^3 cm^{-3} respectively.

Unsaturated hydraulic conductivity versus pressure head

The unsaturated hydraulic conductivity is therefore represented as a function of the negative pressure head (K(h)) or as a function of water content (K(θ)). Substitution of parameters α, 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 graphical representation of Mualem's model (1976) (Fig 3).

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 0.0238 cm min^{-1} (34.27 cm day^{-1}) through inverse modeling using HYDRUS-1D. Data depicted in (Fig 3), it was observed that the negative pressure head decreases with an increase in unsaturated hydraulic conductivity. The unsaturated hydraulic conductivity was found to be in the range of 0 to 0.063 cm day^{-1}, which is much smaller than saturated hydraulic conductivity.

Correlation matrix

The correlation matrix obtained for residual water content, θ_r (cm^3 cm^{-3}), saturated water content, θ_s(cm^3 cm^{-3}), inverse of the air entry value α, (cm^{-1}), parameter *n* in the soil water retention function, saturated hydraulic conductivity K_s, (cm min^{-1}) and pore connectivity parameter (l) is shown in (Table 5).

The parameters *n* and α have the highest correlation coefficient of 0.9814 significantly negative correlation was observed between *α* and θ_s (Table 5). High correlation causes underestimation of parameter uncertainty, slows down convergence rate and increases non-uniqueness. It is expected that the number of highly correlated parameters increases as the number of fitted parameters increases. As a result, the available information in the objective function is reduced.

Table 5 Correlation table for optimized parameters by HYDRUS-1D

	θ_r	θ_s	α	*n*	K_s	l
θ_r	1					
θ_s	0.8238	1				
A	-0.44	-0.8706	1			
N	-0.5926	-0.9445	0.9814	1		
K_s	0.1887	0.1364	-0.0411	-0.0745	1	
L	0.0805	0.0935	-0.0486	-0.0747	0.7945	1

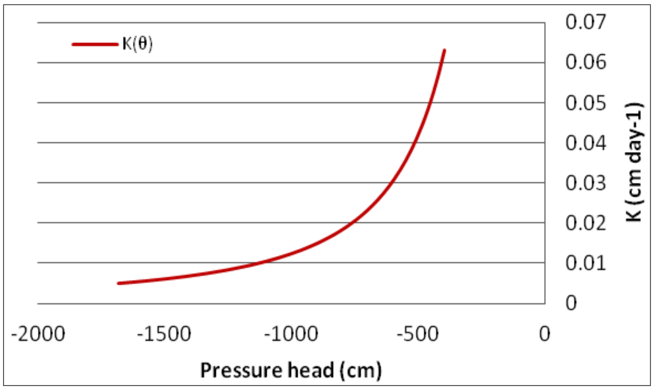

Fig 3 Unsaturated hydraulic conductivity vs. pressure head curve

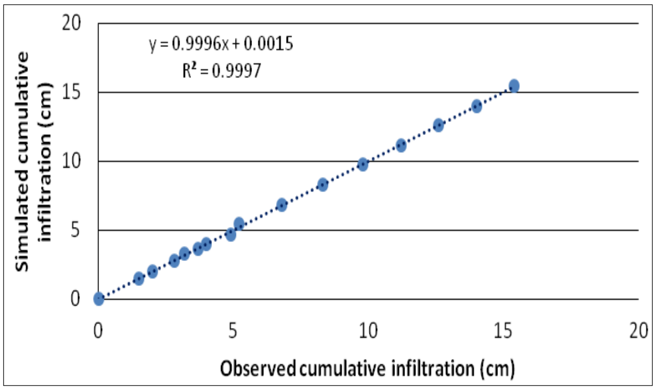

Fig 4 Correlation between observed and simulated cumulative infiltration depth

Table 6 Goodness of fit

Parameter	RMSE (cm)	R^2	MF
	0.003	0.99	0.99

The model performance was evaluated by comparing observed and HYDRUS-1D simulated cumulative infiltration depth using various quantitative measures of error, such as the root mean square error, correlation coefficient, and model efficiency. The correlation between observed and simulated cumulative infiltration was shown in (Fig 4). The performance indicators of overall observed and simulated values of cumulative infiltration depth were presented in (Table 6).

HYDRUS-1D model was used to simulate water infiltration through double ring infiltrometer into a sandy loam soil. The results showed that the numerical inverse solution of double ring infiltrometr data provided a relatively simple method for determining the soil hydraulic parameters. The optimized soil hydraulic parameters were residual water content, (θ_r = 0.0076 cm^3 cm^{-3}), saturated water content, (θ_s = 0.3103 cm^3 cm^{-3}), inverse of the air entry value (α = 0.0011 cm^{-1}), parameter *n* in the soil water retention function (n=1.337), saturated hydraulic conductivity (K_s=0.0238 cm min^{-1}) and pore connectivity parameter, (*l*=0.0011) respectively. The unsaturated hydraulic conductivity was found to be in the range of 0 to 0.063 cm day^{-1}. The root means square error, correlation coefficient, and model efficiency was found as 0.003 cm, 0.99 and 0.99 respectively. From the results, it was concluded that the HYDRUS-1D model is a very good tool for simulating water flow as well as optimization of soil hydraulic parameters through an inverse solution.

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