Fitting Performance of Empirical and Theoretical Soil Water Retention Functions and Estimation of Statistical Pore-Size Distribution-Based Unsaturated Hydraulic Conductivity Models for Flood Plain Soils

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Abstract –For identifying the soil water retention function for its best fitting performance, the empirical retention functions of Brooks-Corey, Van Genuchten and theoretical Kosugi were parameterized for the clay loam and silt loam flood plain soils. The parameters using non-linear least- squares optimization technique as used in the RETC code were optimized and these were used in the Mualem's statistical pore-size distribution-based unsaturated hydraulic conductivity models. It was observed that the log-normal function of Kosugi gave an excellent fitting performance having the highest co-efficient of determination and the lowest residual sum of squares. The physically-based Kosugi function was observed to be followed by empirical functions of Van Genuchten and Brooks-Corey in their fitting performances, respectively

Keywords—Soil water retention functions-Brooks-Corey, van Genuchten, Kosugi, RETC computer code, parameterization, fitting performance, Mualem-based hydraulic conductivity models, model estimation.

INTRODUCTION

Modeling of water dynamics within the partially-saturated soil profile of a specific textural class requires knowledge of the related soil hydraulic characteristics viz: soil water retention functions and soil hydraulic conductivity models and has applications in analyzing the hydrological, environmental and solute transport processes within the soil profile. Different functions have been proposed by various investigators and were reviewed [1]. For estimation of these functions, direct and indirect methods have been employed and in 2005 these have been discussed by Durner and Lipsius [2]. They reported that the direct measurement of unsaturated hydraulic conductivity is considerably more difficult and less accurate and they further suggested the use of indirect method using easily measured soil water retention data from which soil water retention functions can be developed. These retention functions, either empirical or theoretical expressions, fitting the observed soil water retention data to different extents having the specific number of parameters are further embedded into the statistical pore-size distribution-based relative hydraulic conductivity models to develop corresponding predictive theoretical unsaturated hydraulic conductivity models having the same parameters as in the corresponding soil water retention functions given the saturated hydraulic conductivity and the related tortuosity factor. The estimation of the parameters of the retention functions is, therefore, important. In 2012 Solone, et al. [3] reported that the parameterization of the soil water retention functions can be obtained by fitting the function to the observed soil water retention data using the least-squares non-linear fitting algorithms or employing the inverse methods in which the function parameters are iteratively changed so that a given selected function approximates the observed response or using the pedotransfer functions which are regression equations.

Scarce information is available about the parameterization of these functions and the extent of fitting performance of various empirical and theoretical soil water retention functions and subsequently based on these parameters the hydraulic conductivity models for the flood plain soils which constitute mainly the clay loam and silt loam soils need to be estimated. So, in this study, the parameterization of empirical and theoretical soil water retention functions fitting the observed data of these soils has been made to identify suitable functions and further to estimate the unsaturated hydraulic conductivity models based on the estimated parameters for identifying the appropriate models of unsaturated hydraulic conductivity for further use in the modeling of soil water dynamics.

Materials and Methods

Soil water retention data

The average soil water retention data [4] for the soil water suction heads of 100, 300, 1000, 2000 , 3000 , 5000 , 10000 and 15000 cm of different soil samples from the soil profiles (depth 150 cm) of silt loam (percentage of sand, silt and clay: 58.6, 21.9, 14.6, respectively) and clay loam (percentage of sand, silt and clay ranging from 38.3 to 37.4, 20.5 to 24.3 and 34.2 to 37.6, respectively) soils of the flood plains of a seasonal river Ghaggar flowing through a part of Rajasthan was utilized for estimating the parameters of the soil water retention functions described below.

Soil water retention functions

The empirical soil water retention functions proposed by van Genuchten in 1980 [5] with independent m and n of each other and fixed (m = 1-1/n) shape parameters, by Brooks-Corey in 1964 [6] and the statistical pore-size distribution-based soil water retention function by Kosugi in 1996 [7] were used for parameterization. The van Genuchten proposed the sigmoidal- shaped continuous (smooth) five-parametric power-law function as:

$$\theta(h) = \theta_r + (\theta_s - \theta_r)[1 + (\propto_{VG}\ h)^n]^{-m} \quad \textbf{(1)}$$

Where θ is the soil water content at the soil water suction head h and θ_s and θ_r are the residual and saturated soil water contents, respectively. The parameter $\propto_{VG}$ is an empirical constant$[L^{-1}]$. In this function the five unknown parameters are θ_r, θ_s, $\propto_{VG}$, n and m when the shape parameters n and m are independent of each other and when n and m are fixed then these unknown parameters reduced to four. The dimensionless parameters n and m are the parameters related to the pore-size distribution affecting the shape of the function. However, Durner reported that the constraint of fixed condition eliminated some of the flexibility of the function [8].

Brooks –Corey proposed the following empirical four-parametric power-law soil water retention function as:

$$\theta(h) = \theta_r + (\theta_s - \theta_r)(\propto_{BC}\ h)^{-\lambda_{BC}} \quad \textbf{(2)}$$

Where $\propto_{BC}$ is an empirical parameter$[L^{-1}]$ which represents the desaturation rate of the soil water and is related to the pore-size distribution and whose inverse is regarded as the reciprocal of the height of the capillary fringe. The parameter λ_{BC} is the pore-size distribution index affecting the slope of this function and characterizes the width of the pore-size distribution. In this function, the four unknown parameters are θ_r , θ_s, $\propto_{BC}$ and λ_{BC}.

In 1994, Kosugi [9] assumed that the soil pore-size is a log-normal random variable and based on this hypothesis he derived physically-based three-parameter model for the soil water retention function; the three parameters being the mean, variance of the pore-size distribution and the maximum pore radius. In the limiting case, where the maximum pore radius becomes infinite, the three-parameter model simplifies to two-parameter model and based on this simplification Kosugi in 1996 improved the function by developing a physically-based (theoretical) two-parameter log-normal analytical model based on the log-normal distribution density function of the pore radius for the soil water retention as:

$$\theta\,(h) = \theta_r + (\theta_s - \theta_r)\quad \frac{1}{2}\,\mathrm{erfc}\left[\frac{\ln\,(h) - \ln\,(h_m)}{\sqrt{2}\ \sigma}\right] \mathbf{(3)}$$

Where the parameters ln (h_m) and σ denote the mean and standard deviation of ln (h), respectively. The function erfc denotes the complementary error function [10].

Parameter estimation of soil water retention functions

For estimation of unknown parameters of these functions, RETC (RETention Curve) computer code [11] was used by utilizing the soil water retention data only. These unknown parameters were represented by a vector **b** consisting of to $\theta_r, \theta_s, \propto_{VG,}$ n , m for independent shape parameters and $\theta_r, \theta_s, \propto_{VG,}$ n for fixed shape parameters for van Genuchten function and for Brooks-Corey function the vector **b** represented unknown parameters $\theta_r, \theta_s, \propto_{BC,}\ \lambda_{BC}$. For Kosugi function, the vector **b** represented the unknown parameters $\theta_r, \theta_s, h_m, \sigma$ .These parameters were optimized iteratively by minimizing the residual sum of squares (RSS) of the observed and fitted soil water retention data θ(h) and the RSS was taken as the objective function O (**b**) which was minimized by means of a weighted non-linear least-squares optimization approach based on the Marquardt-Levenberg's maximum neighborhood method [12] as:

$$\mathrm{O}\,(\mathbf{b}) = \sum_{i=1}^{N}\left[w_i\{\theta_i - \hat{\theta}_i(\mathbf{b})\}\right]^2 \mathbf{(4)}$$

Where θ_i and $\hat{\theta}_i$ are the observed and the fitted soil water contents, respectively. N is the number of the soil water retention points and equal to 8 in this analysis. The weighting factors w_i , which reflects the reliability of the measured individual data, were set equal to unity in this analysis as the reliability of all the measured soil water retention data was considered equal. A set of appropriate initial estimates of these unknown parameters was used so that the minimization process converges fast after certain iterations to the optimized values of these parameters.

The goodness of fit of the observed and fitted data was characterized by the coefficient of determination (r^2) which measures the relative magnitude of the total sum of squares associated with the fitted function as:

$$r^2 = \sum\left(\hat{\theta}_i - \bar{\theta}_i\right)^2 / \sum(\theta_i - \bar{\theta}_i)^2 \mathbf{(5)}$$

Where $\bar{\theta}_i$ is the mean of observed soil water content data.

The soil water retention functions for these soils were identified in order of superior fitting performance having comparatively higher coefficient of determination (r^2) and lower residual sum of squares (RSS) for the observed and predicted soil water retention data.

Estimation of hydraulic conductivity models

For predicting the unsaturated hydraulic conductivity from the measured soil water retention data, approaches were developed based on the capillary-bundle theory by Childs and Collis-George in 1950 [13], Burdine in 1953 [14] and Mualem in 1976 [15]. In this analysis the widely used Mualem approach was used.

Mualem developed a relative hydraulic conductivity model based on the capillary theory which assumes that the pore radius is inversely proportional to the suction head (h) at which the pore drains and conceptualized the pores as the pairs of capillary tubes whose lengths are proportional to their radii and the conductance of each capillary-tube pair is determined according to the Poiseuille's law (Poiseuille's law states that the flow rate per unit cross-sectional area of a capillary tube is proportional to the square of the radius). He derived the model for the prediction of the relative unsaturated hydraulic conductivity from the soil water retention function. He incorporated the statistical model based on some assumptions. One of these assumptions is that the pore size of a particular radius is randomly distributed in the porous media and another assumption is to incorporate the average flow velocity given by the Hagen-Poiseuille's formulation. He developed the relative hydraulic conductivity model as:

$$K_r(h) = S_e^{l}\left[\frac{\int_{\theta_r}^{\theta}[h(\theta)]^{-1}d\theta}{\int_{\theta_r}^{\theta_s}[h(\theta)]^{-1}d\theta}\right]^2 \quad \textbf{(6)}$$

Where S_e $[= (\theta - \theta_r) / (\theta_s - \theta_r)]$ is the dimensionless effective saturation. The parameter l is the tortuosity factor. $K_r(S_e)$ (= K $(S_e)/K_s$) is the relative unsaturated hydraulic conductivity and K_s is the saturated hydraulic conductivity measured independently. Black reported that the Mualem model to predict the relative hydraulic conductivity from the behavior of the measured soil water retention data is most commonly employed to obtain closed-form analytical expression of unsaturated hydraulic conductivity [16].

Coupling the Brooks-Corey soil water retention function with the Mualem model of relative hydraulic conductivity, the corresponding h-based relative hydraulic conductivity function is expressed as:

$$k_r(h) = (\propto_{BC}\ h)^{-[\lambda_{BC}(l+2)+2]} \quad \textbf{(7)}$$

For developing the closed- form model of the hydraulic conductivity the van Genuchten soil water retention function was coupled with the relative hydraulic conductivity model of Mualem. The condition of fixed shape parameter m = 1-1/n needs to be satisfied for developing the closed form. Embedding the soil water retention function of van Genuchten into the Mualem model resulted into the following corresponding h-based relative hydraulic conductivity model in the closed-form for the condition m = 1 − 1/n as:

$$K_r(h) = \frac{\left[1-(\propto_{VG}\ h)^{n-1}(1+(\propto_{VG}\ h)^n)^{-m}\right]^2}{[1+(\propto_{VG}\ h)^n]^{l\,m}} \quad \textbf{(8)}$$

Kosugi developed a two-parameter hydraulic conductivity model using the corresponding soil water retention function in the Mualem model as:

$$K_r\,(h) = S_e^l\left[\frac{1}{2}\,\mathrm{erfc}\left\{\frac{\ln\,(h/h_m)}{\sqrt{2}\;\;\sigma} + \frac{\sigma}{\sqrt{2}}\right\}\right]^2 \quad \textbf{(9)}$$

The value of tortuosity factor (l) equal 0.5 as reported by Mualem was used in this analysis. The optimized parameters were used in these hydraulic conductivity models for estimation of unsaturated hydraulic conductivity of these soils for further use in modeling the soil water dynamics

Results and Discussion

It is observed from Table 1 that the clay loam flood plain soil having comparatively more clay content was found to have less value of $\propto_{BC}$ in comparison to that for the silt loam flood plain soils indicating more height of the capillary fringe in the clay loam soil as the inverse of $\propto_{BC}$ represents the height of capillary fringe. Kalane et al. also observed more height of the capillary fringe as the clay content in the soil increases [17]. The values of $\propto_{BC}$ of the clay flood plain soil and silt loam flood plain soil were observed to the more or less the same i.e. these values were observed 0.21325 and 0.2025, respectively indicating that the slope of the soil water retention curve is more or less the same for these soils.

In 2002, Kosugi et al. reported that theoretically λ_{BC} value approaches infinity for a porous medium with a uniform pore-size distribution, where as its value approaches a lower limit of zero for soils with a wide range of pore sizes [18]. They reported λ_{BC} value in the range 0.3 to 10.0 while in 2013, Szymkiewicz reported that these values generally ranged from 0.2 to 5.0 [19]. Zhu and Mohanty [20] also reported that the soil water retention function of Brooks and Corey was successfully used to describe the soil water retention data for the relatively homogeneous soils, which have a narrow pore-size distribution with a value for λ_{BC} = 2. Nimmo [21] reported that a medium with many large pores will have a retention curve that drops rapidly to low water content even at low suction head and conversely, a fine-pored medium will retain even at height suction so will have a flatter a retention curve.

Table 1. Optimized parameters of the soil water retention functions for clay loam and silt loam soils of flood plain.

Flood plain soil (clay loam)			
Soil water retention function	**Optimized parameters**		
	$\propto_{VG}/\propto_{BC}$ **(1/ cm)**	n/λ_{BC} **(−)**	**m (−)**
Brooks-Corey	0.00730	0.21325	–
Van Genuchten			
Independent m , n	0.00799	1.005	0.2427
Fixed m = 1- 1/n	0.00746	1.2378	–

Kosugi	h_m = 507.29 cm	σ = 4.4236 cm	
Flood plain (Silt loam)			
Brooks-Corey	0.0219	0.2025	–
Van Genuchten Independent m , n Fixed m = 1- 1/n	 0.00497 0.00521	 1.005 1.2575	 0.2690 –
Kosugi	h_m = 1232.78 cm	σ = 3.6815 cm	-

In the van Genuchten function, when the factor one is disregarded ($\alpha_{VG} h^n \gg 1$) then it becomes a limiting case and is approximated to the Brooks-Corey function and the product of m and n in the van Genuchten function become equal to λ_{BC} of the Brooks-Corey function. The product of m and n remains constant and for that if n is increased then m must be simultaneously decreased. For the fixed case i.e. m = 1-1/n, the parameter λ_{BC} should be equal to n – 1. The properties of the soil media which are described by the two parameters ($\propto_{BC}, \lambda_{BC}$) in the Brooks-Corey model are described by three parameters ($\propto_{VG}, n, m$) in the van Genuchten model. From Table 1 it is observed that for the case of van Genuchten function with independent shape parameters (m , n) and fixed shape parameters m = 1-1/n, the value of α_{VG} was observed to be higher for clay loam soil (fine-textured) than the silt loam soil which is comparatively medium- textured. The same observation was reported by Jauhiainen [22].

It is observed from Table 2 that the log-normal function of Kosugi gave an excellent description of the observed soil water retention data having the highest r^2 = 0.9969 and the lowest RSS = 0.00016 for clay loam soil and r^2 = 0.9932 and RSS = 0.00033 for silt loam soil followed by the van Genuchten function with independent shape parameters which yielded r^2 = 0.9929 and RSS = 0.00038 for clay loam soil and r^2 = 0.9864 and RSS = 0.00066 for silt loam soil. Among the van Genuchten functions, the function with fixed shape parameters yielded higher RSS (13.16 to 15.15 percent) for these soils. The non-linear least-squares fitting of the Brooks-Corey function resulted in the least value of r^2 = 0.9881 and the highest value of RSS = 0.00063 for clay loam and r^2 = 0.9724 and RSS = 0.00135 for silt loam soils of flood plain showing that Brooks-Corey function followed the van Genuchten function in its fitting performance and for these soils performed comparatively better in the clay loam. All the soil water retention functions gave comparatively better fitting performance for the clay loam flood plain soil in comparison to silt loam flood plain soil.

Table 2.Statistics of the fitting performance of the soil water retention functions.

Soil water retention function	**Flood plain soil (clay loam)**		**Flood plain soil (silt loam)**	
	RSS (10^{-5})	$\mathbf{r^2}$	**RSS** (10^{-5})	$\mathbf{r^2}$
Brooks-Corey	63	0.9881	135	0.9724

Van Genuchten Independent m , n Fixed m = 1- 1/n	 38 43	 0.9929 0.9919	 66 76	 0.9864 0.9843
Kosugi	16	0.9969	33	0.9932

The physically-based log-normal function of Kosugi gave the best fitting performance followed by empirical van Genuchten and Brooks-Corey functions in order of superior fitting performance for embedding in the statistical pore-size distribution-based Mualem's relative hydraulic conductivity model for developing the unsaturated hydraulic conductivity function for modeling the soil water dynamics in these flood plain soils. The log-normal function of Kosugi has a merit in that it is a theoretically derived function, and therefore, the physical meaning of each parameter is clearly defined.

However, for optimizing the parameters of the soil water retention functions, the number of fitted parameters must be reduced in order to minimize the non-uniqueness of the optimized parameters and efforts should be made to independently measure the parameters such as the saturated soil water contentθ_s. The assumed value of residual soil water content θ_r can also be used as its measurement is extremely difficult in the laboratory. This will further reduce the number of parameters to be optimized. It is also observed that the soil water retention functions under study predict infinite value of the soil water suction head (h) as the effective saturation (S_e) approaches zero which is not consistent with the fact that even under oven-dry condition the soil water suction has a finite value. So, therefore, these functions should be used in the range of effective saturation significantly larger than zero.

Conclusion

The parameters of empirical soil water retention functions of Brooks-Corey and Van Genuchten and the theoretical soil water retention function of Kosugi were optimized using non-linear least- squares optimization algorithm as used in the RETC computer code for the clay loam and silt loam flood plain soils. These parameters were used in the Mualem's statistical pore-size distribution-based models for estimation of corresponding unsaturated hydraulic conductivity models. The log-normal function of Kosugi gave an excellent fitting performance with highest co-efficient of determination and the lowest residual sum of squares equal for these soils. The physically-based Kosugi function was observed to be followed by empirical functions of Van Genuchten and Brooks-Corey in their fitting performances. It is proposed that theoretical Kosugi model of unsaturated hydraulic conductivity can be used for mathematical simulation studies of soil water dynamics.

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