Research Article

Parameterization and Fitting Performance of Soil Water Retention Functions using Non-linear Least-Squares Optimization for Aeolian Soils

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ABSTRACT

The empirical soil water retention functions of Campbell, Brooks-Corey and van Genuchten for their fitting performance were parameterized for the desert plains (loamy sand) and dunal (sandy loam) soils. The parameters were optimized using non-linear least-square technique as used in the RETC code. It was observed that the van Genuchten with fixed shape parameters (m = 1-1/n) and Brooks-Corey function gave excellent fitting performances having the highest coefficients of determination and the lowest residual sum of squares followed by van Genuchten function with independent shape parameters for dunal soil. Both van Genuchten with fixed shape parameters (m = 1-2/n) and Campbell functions performed less in comparison to other functions. All these functions showed better performance for dunal soils in comparison to desert plains. The optimized parameters of these functions were proposed to be used in the Burdine and Mualem's statistical pore-size distribution models for estimation of unsaturated hydraulic conductivity functions.

Key words: Soil water retention functions, RETC code, Parameterization, Fitting performance, Hydraulic conductivity functions, Aeolian soils

Introduction

Knowledge of soil hydraulic functions is important for modeling the storage, movement, redistribution of water and solute transport within the unsaturated soil profile of a particular textural class. Different hydraulic functions have been proposed by various investigators (Leij *et al.*, 1997 and Too *et al.*, 2014). For estimation of hydraulic conductivity functions, direct and indirect methods have been employed and these have been reviewed by Durner and Lipsius (2005). 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 fitting the observed soil water retention data to different extents having the specific number of parameters can be further embedded into the statistical pore-size distribution-based relative hydraulic conductivity models of either Burdine (1953) or Mualem (1976) for developing the corresponding predictive theoretical unsaturated hydraulic conductivity functions having the same parameters as in the corresponding soil water retention functions given the related saturated hydraulic conductivity and the tortuosity factor. The estimation of the parameters of the soil water retention functions is, therefore, important. Solone *et al.* (2012) reported that the parameterization of the soil water retention functions can be obtained

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by (a) fitting the function to the observed soil water retention data using the least-squares non-linear fitting algorithms, (b) employing inverse methods in which function parameters are iteratively changed so that a given selected function approximates the observed response or (c) using pedotransfer functions which are regression equations.

Scarce information is available on the evaluation of these parameters and the fitting performance of empirical soil water retention functions. The estimates of theoretical-based unsaturated hydraulic conductivity functions for the aeolian soils are also limited. These soils constitute mainly the desert plains and dunal soils forming large tracts of cultivable land in Rajasthan and adjoining area of Haryana. In these regions, rainwater harvesting and water management technologies in command areas can be evaluated using the soil water dynamics modeling for which information on hydraulic functions is needed. In this study, the parameterization and the fitting performance of the soil water retention functions of these soils has been made to identify suitable functions and subsequently to estimate the unsaturated hydraulic conductivity functions based on the optimized parameters for further use in the modeling of soil water dynamics.

Materials and Methods

Soil water retention data

Soil water retention data (Yadav *et al*., 1995) for 100, 300, 1000, 2000, 3000, 5000, 10000 and 15000 cm suction heads of aeolian soils (depth 150 cm) were used in the study. These soils include desert plain soils (loamy sand with sand, silt and clay percentages ranging from 81.4 to 85.9, 3.7 to 5.0 and 6.9 to 8.4, respectively) and dunal soils (sandy loam with sand, silt and clay percentages ranging from 72.5 to 80.3, 6.0 to 10.0 and 11.8 to 16.1, respectively).

Soil water retention functions

The empirical soil water retention functions proposed by van Genuchten (1980) with

independent m and n and fixed (m = 1-1/n and m = 1-2/n) shape parameters, Campbell (1974) and Brooks-Corey (1964) were used for parameterization and fitting performance. Van Genuchten (1980) proposed the sigmoidal-shaped continuous (smooth) five-parametric power-law function as:

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

where θ is the soil water content at the soil water suction head h and θ_r and θ_s are the residual and saturated 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 either as m = 1 - $^1/_n$ or m = 1 - $^2/_n$. The shape parameters are related to the pore-size distribution affecting the shape of the function. For developing the closed-form function of hydraulic conductivity by coupling the van Genuchten soil water retention function with the relative hydraulic conductivity models either of Burdine (1953) or Mualem (1976), the conditions of fixed shape parameters m = 1 - $^2/_n$ and m = 1 - $^1/_n$ need to be satisfied to make the conductivity function in the closed form, respectively. However, Durner (1994) reported that these constraints eliminated some of the flexibility of the functions.

Brooks and Corey (1964) proposed the following empirical four-parametric power-law soil water retention function as:

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

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. The 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}.

Campbell (1974) proposed the empirical three-parametric power-law soil water retention function as:

$$\theta\,(h) = \theta_s(\propto_{CA}\,h)^{\lambda_{CA}} \qquad (3)$$

This function was derived from the Brooks and Corey model (1964) with residual water content (θ_r) equal to zero. The parameters $\propto_{CA}$ and λ_{CA} have the same meaning as $\propto_{BC}$ and λ_{BC} in the Brooks-Corey function. In this function, the three unknown parameters are θ_s, $\propto_{CA}$ and λ_{CA}.

Parameter estimation and fitting performance of soil water retention functions

For estimation of unknown parameters of these functions, RETC (Retention Curve) computer code (van Genuchten *et al.*, 1991) was used by utilizing the soil water retention data only. The unknown parameters of these functions were represented by a vector b. These parameters were optimized iteratively by minimizing the residual sum of squares (RSS) of the observed and fitted soil water retention data (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 (Marquardt, 1963) as:

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

where θ_i are $\hat{\theta}_i$ the observed and the fitted soil water contents, respectively; N is the number of soil water retention points (8 in this analysis). The weighting factor 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 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 measured the relative magnitude of the total sum of squares associated with the fitted function as:

$$r^2 = \sum\big(\hat{\theta}_i - \bar{\theta}_i\big)^2 / \sum(\theta_i - \bar{\theta}_i)^2 \qquad (5)$$

where $\bar{\theta}_i$ is the mean of observed data.

Estimation of hydraulic conductivity functions

Based on the statistical pore-size distribution, the relative hydraulic conductivity function due to the capillary flow is defined by a mathematical expression (Zhang *et al.*, 2003) as:

$$K_r(h) = S_e^{l}\left[\frac{\int_{\theta_r}^{\theta}[h\,(\theta)]^{-\beta}\,d\theta}{\int_{\theta_r}^{\theta_s}[h\,(\theta)]^{-\beta}\,d\theta}\right]^{\gamma} \qquad (6)$$

where S_e [$= (\theta - \theta_r)/(\theta_s - \theta_r)$] is the dimensionless effective saturation. The parameter l is the tortuosity factor and β and γ are the constants. Eq. (6) reduces to the Burdine model (1953) when $\beta = 2$ and $\gamma = 1$, and to the Mualem model (1976) when $\beta = 1$ and $\gamma = 2$. $K_r(S_e)$ ($= K(S_e)/K_s$) is the relative unsaturated hydraulic conductivity and K_s [LT^{-1}] is the saturated hydraulic conductivity measured independently.

Coupling the Brooks-Corey soil water retention function with the Burdine and Mualem models of relative hydraulic conductivity, the corresponding h-based relative hydraulic conductivity functions were expressed as:

$$k_r(h) = (\propto_{BC}\,h)^{-[\lambda_{BC}(l+1)\,+\,2]} \qquad (7)$$

$$k_r(h) = (\propto_{BC}\,h)^{-[\lambda_{BC}(l+2)\,+\,2]} \qquad (8)$$

Embedding the soil water retention function of van Genuchten into the Burdine and Mualem models resulted into the following corresponding h-based relative hydraulic conductivity functions in the closed-form for the conditions m = 1- 2/n for Burdine and m = 1-1/n for Mualem models, respectively as:

$$K_r(h) = \frac{\left[1 - (\propto_{VG}\,h)^{n-2}(1 + (\propto_{VG}\,h)^n)^{-m}\right]}{[1 + (\propto_{VG}\,h)^n]^{l\,m}} \qquad (9)$$

$$K_r(h) = \frac{\left[1 - (\propto_{VG}\,h)^{n-1}(1 + (\propto_{VG}\,h)^n)^{-m}\right]^2}{[1 + (\propto_{VG}\,h)^n]^{l\,m}} \qquad (10)$$

The values of tortuosity factor (l) equal to 2.0 and 0.5 as proposed by Burdine (1953) and Mualem (1976) were used in this analysis for Burdine and Mualem-based relative hydraulic conductivity functions, respectively.

Table 1. Optimized parameters of the soil water retention functions for desert plain and dunal soils

Soil water retention function	Optimized parameters		
	$\alpha_{VG}/\alpha_{CA}/\alpha_{BC}$ (1/ cm)	$n/\lambda_{CA}/\lambda_{BC}$ (–)	m (–)
Desert plain soil (Loamy sand)			
Campbell	0.1903	0.2623	–
Brooks-Corey	0.1559	0.3418	–
van Genuchten			
Independent m , n	0.6191	1.4138	0.2433
Fixed m = 1- 1/n	0.5493	1.3427	–
Fixed m = 1- 2/n	0.5828	2.3421	–
Dunal soil (Sandy loam)			
Campbell	0.0902	0.2741	–
Brooks-Corey	0.0784	0.3418	–
van Genuchten			
Independent m , n	0.2525	1.3768	0.2499
Fixed m = 1- 1/n	0.2251	1.3448	–
Fixed m = 1- 2/n	0.5906	2.2742	–

Results and Discussion

It is seen from Table 1 that the dunal soil (sandy loam) having comparatively more clay and silt contents had smaller values of α_{VG} for independent and fixed (m = 1-1/n) shape parameters of van Genuchten functions in comparison to those for the desert plain soils (loamy sand). The same trend was observed for parameters α_{CA} of Campbell and α_{BC} of Brooks-Corey functions indicating more height of the capillary fringe (inverse of α_{BC} or α_{CA}) in the sandy loam soil in comparison to that in the loamy sand soil. Kalane *et al*. (1994) also observed that the sandy loam soil has more height of the capillary fringe in comparison to that in the loamy sand soil. Among the Campbell and Brooks-Corey functions, the values of λ_{CA} ranged from 0.2623 to 0.2741 for both the soils and were observed to be less than λ_{BC} (0.3418) for both the soils indicating that the slope of these soil water retention function (curve) of Brooks-Corey was observed to be more. Kosugi *et al*. (2002) reported that theoretically λ_{BC} value approached infinity for a porous medium with a uniform pore-size distribution, whereas its value approaches a

lower limit of zero for soils with a wide range of pore sizes. They reported λ_{BC} value in the range 0.3 to 10.0 while Szymkiewicz (2013) reported that these values generally ranged from 0.2 to 5.0. Zhu and Mohanty (2003) also reported that the soil water retention of Brooks and Corey was successfully used to describe the retention data for the relatively homogeneous soils, which have a narrow pore-size distribution with a value for λ_{BC} = 2. Nimmo (2005) 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-pore medium will retain even at high suction so will have a flatter retention curve.

In the van Genuchten function, when the factor one is disregarded ($\alpha_{VG}h^n \gg 1$ under comparatively drier conditions) then it becomes a limiting case and can be approximated to the Brooks-Corey function. Under this condition, the product of m and n in the van Genuchten function becomes equal to λ_{BC} of the Brooks-Corey function. For the product mn to remain constant, if n is increased then m simultaneously must be decreased. For the fixed cases i.e. m = 1-1/n and

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

Soil water retention function	Desert plain soil (loamy sand)		Dunal soil (sandy loam)	
	RSS (10⁻⁵)	r²	RSS (10⁻⁵)	r²
Campbell	14	0.9851	6	0.9966
Brooks-Corey	12	0.9871	3	0.9986
van Genuchten				
Independent m, n	12	0.9876	3	0.9980
Fixed m = 1- 1/n	12	0.9876	3	0.9986
Fixed m = 1- 2/n	12	0.9876	6	0.9966

$m = 1 - {}^2/_n$, the parameter λ_{BC} should be equal to n-1 and n-2, respectively. In these functions, the hydraulic properties of the soil media, are described by the combined effects of two parameters ($\alpha_{BC}, \lambda_{BC}$) in the Brooks-Corey function and by three parameters (α_{VG}, n, m) in the van Genuchten function. From Table 1 it is observed that for the case of van Genuchten function with independent shape parameters (m,n) and fixed (1-1/n) shape parameters, the value of α_{VG} was observed to be higher for loamy sand (coarse-textured soil) than that of sandy loam soil which is comparatively medium- textured.

Table 2 shows that all the functions give better fitting performance for the dunal soils as indicated by higher r² and lower RSS values in comparison to those for the desert plain soils. Within the dunal soil, comparatively better predictions were equally given by Brooks-Corey and van Ganuchten functions with independent shape parameters and fixed (m = 1 - ¹/ₙ) shape parameters in comparison to the Campbell function or the van Genuchten function with fixed (m = 1 - ²/ₙ) shape parameters. For the desert plain soil, Campbell function gave comparatively lesser fit (with least value of r² equal to 0.9851 and highest value of RSS equal to 14 × 10⁻⁵) to the measured soil water retention data in comparison to other functions. Mayr and Jarvis (1999) reported that the van Genuchten function gave adequate fitting performance to the measured soil water contents across a wide range of suction heads. Assouline and Tartakovsky (2001) also reported that among a variety of soil water retention functions, the functions proposed by

Brooks-Corey (1964) and van Genuchten (1980) gave better predictions. Mavimbela and van Rensburg (2013) also parameterized the soil water retention functions of Brooks-Corey (1964) van Genuchten (1980) using RETC code (van Genuchten *et al.*, 1991) and reported that these functions fitted the measured soil water retention data with coefficient of determination (r²) of no less than 0.98. In this analysis, the most fitted performance was observed to be of the van Genuchten function with fixed shape parameters (m = 1 - 1/n) and the Brooks-Corey function for dunal soil (sandy loam) and least fitted performance by Campbell function. For the desert soil (loamy sand) also, the Campbell function gave the least fitting performance.

The values of the optimized parameters of these soil water retention function were used in the corresponding unsaturated hydraulic conductivity function for describing the soil water behavior. However, it is proposed that 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 parameters such as the saturated soil water content. Also, as the residual soil water content is extremely difficult to determine, it is suggested that its appropriate value may also be specified *a priori* depending upon the soil texture at which the hydraulic conductivity approaches to nearly zero. Though the van Genuchten soil water retention function gave the excellent performance but the use of the corresponding

hydraulic conductivity function for developing analytical models of soil water dynamics is mathematically difficult but it is proposed to be used in the numerical model. For developing the analytical model describing the soil water dynamics, the Campbell's hydraulic conductivity function is preferred as it can be easily analytically integrated.

Conclusion

The van Genuchten with fixed shape parameters (m = 1 - $^1/_n$) and Brooks-Corey soil water retention functions yielded highest fitting performances, followed by van Genuchten function with independent shape parameters for dunal soils. Both van Genuchten with fixed shape parameters (m = 1 - $^2/_n$) and Campbell functions performed less in comparison to other functions. All these functions performed better for the dunal soils in comparison to desert plain soils. The optimized parameters of these functions were proposed for estimation of unsaturated hydraulic conductivity of these soils.

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