

Parameter Optimization and Evaluation of Hydrodynamic Functions in the Wet Range of Water Availability in Different Soils

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Abstract - The knowledge of the soil hydrodynamic functions is essential for modeling the soil water dynamics and different components of water balance. Major contribution of these components occurs during the wet range of water availability in the soil profile. The functional form of the most commonly used theoretical hydrodynamic functions of Brooks-Corey and van Genuchten coupled with Burdine and Mualem hydraulic conductivity models were developed for coarse, medium, and moderately fine-textured soils. For developing these functional forms, parameterization and fitting performance of the corresponding soil water retention functions were performed using RETC computer code employing non-linear least-squares optimization. It was observed that for the wet range of water availability in the loam and silty clay loam soil, the best performance was given by the Brooks-Corey soil water retention function followed by van Genuchten functions with $m = 1 - 1/n$ and $m = 1 - 2/n$. However for this range of water availability, the van Genuchten functions with $m = 1 - 1/n$ gave a slight better performance in sand in comparison to other functions which gave same performance. It was observed that as the sand content of these soils decreases, the hydraulic conductivity and soil water diffusivity at particular soil water content also decreased. The hydraulic conductivity predicted by the Mualem-van Genuchten function were observed to be less than predicted by Mualem-Brooks-Corey function and the same trend was observed for the soil water diffusivity for these soils.

Key Words: Soil water retention functions–Brooks-Corey, van Genuchten, RETC code, parameterization, fitting performance, Burdine and Mualem models, hydraulic conductivity, soil water diffusivity.

INTRODUCTION : The knowledge of hydrodynamic functions of soil water retention, hydraulic conductivity and soil water diffusivity is essential for modeling the different components of the water balance i.e. internal drainage and evaporation from the soil profile, capillary contribution to it and water storage changes within it as well as solute and contaminant transport to and from the groundwater. These processes are affected mainly by the texture and degree of wetness of the soil profile. For in-situ estimation of hydraulic conductivity of the unsaturated soil, direct methods of plane of zero flux [1] constant flux vertical time domain reflectometry [2] and instantaneous profile method [1] were used but Durner and Lipsius [3] reported that these methods are considerably more difficult and less accurate and they further suggested the use of indirect method of estimation using soil water retention function developed from the easily measured soil water retention data. Various soil water retention functions, relation between soil water content and soil water suction head, have been proposed [4,5,6,7,8,9,10,11,12,13,14] Some of these functions though provided better predictions but are difficult to incorporate into the statistical pore-size distribution models for developing the analytical hydrodynamic functions. Abrisqueta et al. [15] reported that there is a wide body of literature in which hydrodynamic behavior of the soils have been described based on their water retention functions for the entire range of saturation. Leij et al. [16] and Assouline and Tartakovsky[17] reported that among a variety of soil water retention functions which were evaluated for the entire range of soil water from saturation to oven- dryness, the functions proposed by Brooks-Corey and van Genuchten are most popular for use in numerical modeling of

water flow and solute transport within the unsaturated porous media. These two empirical retention functions of with specific number of parameters fitting the observed soil water retention data to different extents can be embedded into the statistical pore-size distribution-based hydraulic conductivity models of either Burdine [18] or Mualem [19] for developing the corresponding predictive theoretical unsaturated hydraulic conductivity functions having the same parameters as in the corresponding soil water retention functions and further developing the soil water diffusivity functions. Rossi and Nimmo [13] reported that these soil water retention functions performed differently in the wet, middle and dry ranges of water content from saturation to oven-dryness in the soil profile.

Major contribution of these processes as stated above occur in the moist (wet) range of soil water and such moist conditions prevail for most of the time during the periods immediately following each rainfall event and under drip irrigation. So in this study, the hydrodynamic functions in the wet range of water availability in different soils were evaluated for developing the functional unsaturated hydraulic conductivity and soil water diffusivity functions for further use in modeling the soil water dynamics.

Materials and Methods

Soil water retention data

The soil water retention data Kalane et al., [20] at the soil water suction heads of 0, 20, 40, 60, 80, 100, 120, 150 and 180 cm (taken as positive) of different samples from the soil textural classes of sand (coarse texture), loam (medium texture) and silty clay loam (moderately fine texture) collected from different locations in Haryana, India and the corresponding with the soil water contents were utilized for optimizing the parameters of the soil water retention functions and for evaluating the hydrodynamic functions. According to USDA textural classification of soils, the textural class of sand has proportions of sand, silt and clay ranging from 86 to 100, 0 to 14 and 0 to 10 percent, respectively while these constituents range from 23 to 52, 28 to 50 and 7 to 27 percent in soil, respectively and the silty clay loam soil has these ranging from 0 to 20, 40 to 73 and 27 to 40 percent, respectively.

Soil water retention functions

The empirical soil water retention functions proposed by van Genuchten [7] with fixed ($m = 1 - 1/n$ and $m = 1 - 2/n$) shape parameters and Brooks-Corey [4] were used in this analysis. The van Genuchten proposed the empirical sigmoidal-shaped continuous (smooth) four-parametric power-law function as:

$$S_e = [1 + (\alpha_{VG} h)^n]^{-m} \quad (1)$$

Where $S_e [= (\theta(h) - \theta_r)/(\theta_s - \theta_r)]$ is the dimensionless effective saturation, θ , θ_s and θ_r are the water content at the soil water suction head h , saturated and residual water contents, respectively. The parameter α_{VG} is an empirical constant [L^{-1}]. In this function, the four unknown parameters are θ_r , θ_s , α_{VG} and n . The dimensionless parameters n and m (fixed with each other) are the parameters related to the pore-size distribution affecting the shape of the function. For developing the closed-form (analytical) function of the unsaturated hydraulic conductivity by coupling the van Genuchten soil water retention function with the hydraulic conductivity models of either of Burdine or Mualem, the conditions of fixed shape parameters $m = 1 - 2/n$ and $m = 1 - 1/n$ need to be satisfied, respectively. However, Durner [21] reported that these constraints of fixing the shape parameters eliminated some of the flexibility.

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

$$S_e = (\alpha_{BC} h)^{-\lambda_{BC}} \quad (2)$$

Where α_{BC} is an empirical parameter [L^{-1}] representing desaturation rate of soil water 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 $\theta_r, \theta_s, \alpha_{BC}$ and λ_{BC} .

Estimation of hydraulic conductivity functions

Based on the statistical pore-size distribution in the soil medium, the relative hydraulic conductivity function is defined by a mathematical expression [22] as:

$$K_r(S_e) = S_e^l \left[\frac{\int_{\theta_r}^{\theta} [h(\theta)]^{-\beta} d\theta}{\int_{\theta_r}^{\theta_s} [h(\theta)]^{-\beta} d\theta} \right]^\gamma \quad (3)$$

The parameter l is the tortuosity factor which characterizes the combined effects of pore-connectivity and flow path and β and γ are the constants. Eq. (3) reduces to the Burdine model when $\beta = 2$ and $\gamma = 1$ and to the Mualem model when $\beta = 1$ and $\gamma = 2$. $K_r(S_e) (= K(S_e)/K_s)$ is the dimensionless relative unsaturated hydraulic conductivity and $K_s [LT^{-1}]$ is the saturated hydraulic conductivity.

Coupling of the Brooks-Corey soil water retention function with the Burdine and Mualem models yielded the corresponding S_e - based hydraulic conductivity functions, respectively as:

$$K(S_e) = K_s S_e^{(l+1)+(2/\lambda_{BC})} \quad (4)$$

$$K(S_e) = K_s S_e^{(l+2)+(2/\lambda_{BC})} \quad (5)$$

Van Genuchten coupled his soil water retention function $S_e(h)$ with the Mualem model and its integration led to the derivation of the unsaturated hydraulic conductivity in the form of an Incomplete Beta Function for a general case of independent parameters m and n as:

$$K(S_e) = K_s S_e^l [I_\zeta(m + 1/n, 1 - 1/n)]^2 \quad (6)$$

Where $I_\zeta(m + 1/n, 1 - 1/n)$ is the Incomplete Beta Function and $\zeta = S_e^{1/m}$. Under the condition $m = 1 - 1/n$, the Eq. (6) when integrated, the unsaturated hydraulic conductivity reduced to the closed-form as:

$$K(S_e) = K_s S_e^l \left[1 - \left(1 - S_e^{1/m}\right)^m \right]^2 \quad (7)$$

The Burdine-based hydraulic conductivity function with independent m and n parameters is expressed as:

$$K(S_e) = K_s S_e^l [I_\zeta(m + 2/n, 1 - 2/n)] \quad (8)$$

Where $I_\zeta(m + 2/n, 1 - 2/n)$ is the Incomplete Beta Function and $\zeta = S_e^{1/m}$. The integration of Eq. (8) under the constraint $m = 1 - 2/n$ led to the analytical form of S_e - based unsaturated hydraulic conductivity as:

$$K(S_e) = K_s S_e^l [1 - (1 - S_e^{1/m})^m] \quad (9)$$

Estimation of soil water diffusivity functions

The soil water diffusivity $D(S_e)$ [$L^2 T^{-1}$] was derived by multiplying the $K(S_e)$ by the inverse of the soil water capacity $C(S_e)$ [L^{-1}]. The $C(S_e)$ is the first derivative of the soil water retention function i.e. $d\theta/dh$. For the Brooks-Corey soil water retention function, $C(S_e)$ was derived as:

$$C(S_e) = \alpha_{BC} \lambda_{BC} (\theta_s - \theta_r) S_e^{(\lambda_{BC} + 1)/\lambda_{BC}} \quad (10)$$

Multiplying Eqs. (4) and (5) by the inverse of Eq. (10) resulted in the Burdine and the Mualem-based Brooks-Corey soil water diffusivity functions, respectively as:

$$D(S_e) = K_s [\alpha_{BC} \lambda_{BC} (\theta_s - \theta_r)]^{-1} [S_e^{(1+1/\lambda_{BC})}] \quad (11)$$

$$D(S_e) = K_s [\alpha_{BC} \lambda_{BC} (\theta_s - \theta_r)]^{-1} [S_e^{(1+1/\lambda_{BC})}] \quad (12)$$

For the soil water retention function, the soil water capacity $C(S_e)$ was derived as:

$$C(S_e) = m n \alpha_{VG} (\theta_s - \theta_r) S_e^{(1/m)} [1 - S_e^{1/m}]^m \quad (13)$$

Multiplying Eqs. (7) and (9) by the inverse of Eq. (13) yielded the Mualem and Burdine- based van Genuchten soil water diffusivity functions, respectively as:

$$D(S_e) = K_s \left[\frac{(1-m)}{\alpha_{VG} m (\theta_s - \theta_r)} \right] [S_e^{(1-m)}] \left[(1 - S_e^{1/m})^{-m} + (1 - S_e^{1/m})^m - 2 \right] \quad (14)$$

$$D(S_e) = K_s \left[\frac{(1-m)}{\alpha_{VG} (1+m) (\theta_s - \theta_r)} \right] [S_e^{(1-m)}] \left[(1 - S_e^{1/m})^{-m} - 1 \right] \quad (15)$$

For using the value of tortuosity factor (l), Wosten and van Genuchten [23] reported that this value where is from soil to soil and fits may not be reasonable especially for medium and fine-textured soils. But in this analysis, the average values of tortuosity factor (l) equal to 2.0 and 0.5 as proposed by Burdine and Mualem were used for Burdine and Mualem-based predictive unsaturated hydraulic conductivity and soil water diffusivity functions, respectively. The values of m for the Burdine and Mualem-based of conductivity and diffusivity functions were calculated by fixing $m = 1 - 2/n$ and $m = 1 - 1/n$, respectively. The saturated hydraulic conductivity values as determined experimentally by Kalane et al. [20] for these soils were used.

Parameterization and evaluation of fitting performance

For estimation of unknown parameters of soil water retention functions, RETC (REtention Curve) computer code van Genuchten et al. [24] was used by utilizing the observed soil water retention data only and these were represented by a vector \mathbf{b} equal to $\theta_r, \theta_s, \alpha_{VG}, n$ for van Genuchten function and equal to $\theta_r, \theta_s, \alpha_{BC}, \lambda_{BC}$, for Brooks-Corey function. In this code, these parameters are optimized iteratively by minimizing the residual sum of squares (RSS) of the observed and fitted soil water retention data $\theta(h)$ by

taking RSS as the objective function $O(\mathbf{b})$ using weighted non-linear least-squares optimization approach based on the Marquardt-Levenberg's maximum neighborhood method [25] as:

$$O(\mathbf{b}) = \sum_{i=1}^N [w_i \{\theta_i - \hat{\theta}_i(\mathbf{b})\}]^2 \quad (16)$$

Where θ_i and $\hat{\theta}_i$ are the observed and the corresponding fitted soil water contents, respectively. N is the number of the soil water retention data points and equal to 9 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 after certain iterations to the optimized values of these parameters. For evaluating the fitting performance, goodness of fit of the observed and fitted data was estimated by the coefficient of determination (r^2) characterizing the relative magnitude of the total sum of squares associated with the fitted function as:

$$r^2 = \frac{\sum (\hat{\theta}_i - \bar{\theta}_i)^2}{\sum (\theta_i - \bar{\theta}_i)^2} \quad (17)$$

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

Results and Discussion

The optimized values of saturated water contents (Table 1) were observed to be 0.40, 0.46 and 0.52 cm^3/cm^3 for the sand, loam and silty clay loam soils, respectively for both the soil water retention functions of Brooks-Corey and van Genuchten and on comparison with the experimentally determined saturated water contents Kalane et al. [20] a complete perfect match was found. It was also observed that as the fineness of the soil texture increases, the predicted residual soil water contents increased from 0.02 to 0.25 cm^3/cm^3 by Brooks-Corey function, from 0.04 to 0.35 cm^3/cm^3 by van Genuchten function with constraint $m = 1 - 1/n$ and from 0.03 to 0.33 cm^3/cm^3 by van Genuchten with fixed shape parameter $m = 1 - 2/n$ for these soils. The residual water contents predicted by Brooks-Corey function were observed to be less in comparison to predicted by van Genuchten function. Among the van Genuchten functions, the van Genuchten with fixed $m = 1 - 2/n$ predicted less residual soil water contents in comparison with fixed $m = 1 - 1/n$. The residual water contents predicted by these functions ranged from 0.02 to 0.04, 0.16 to 0.25 and 0.25 to 0.35 cm^3/cm^3 for sand, loam and silty clay loam soils, respectively.

It is seen from Table 1 that as the clay content of these soils increases, the values of α_{BC} and α_{VG} decreased and the Brooks-Corey function predicted α_{BC} values of 0.1062, 0.0452 and 0.0321 for sand, loam and silty clay loam soils, respectively indicating more height of the capillary fringe (inverse of α_{BC}) in the silty clay loam followed by loam and sand soils. These α_{BC} values were observed to be higher than the values of α_{VG} for these soils. Among the van Genuchten functions, α_{VG} values of 0.0712, 0.0254 and 0.0184 predicted with fixed $m = 1 - 1/n$ were found to be lower than function with $m = 1 - 2/n$.

The values of λ_{BC} were observed (Table 1) to be 0.5969, 0.4228 and 0.4225 for sand, loam and silty clay loam soils indicating that as the sand content of these soils decreases, these values also decreased which indicated that the slope of the water retention function of Brooks-Corey was observed to be more in sand in comparison to loam and silty clay loam soils. This showed that the porous medium of sand has comparatively more uniform pore-size distribution. Kosugi et al. [26] also reported that theoretically λ_{BC} value approaches infinity for a porous medium with a uniform pore-size distribution, whereas its value approaches a lower limit of zero for soils with a

Table 1. Optimized values of the parameters of the soil water retention functions for different soils

Sand (Coarse texture)				
Soil water retention function	Optimized values of parameters			
	θ_r (cm ³ /cm ³)	θ_s (cm ³ /cm ³)	α_{VG}/α_{BC} (1/cm)	n/λ_{BC} (-)
Brooks-Corey	0.02	0.40	0.1062	0.5969
Van Genuchten				
Fixed $m = 1 - 1/n$	0.04	0.40	0.0712	1.8595
Fixed $m = 1 - 2/n$	0.03	0.40	0.0936	2.6773
Loam (Medium texture)				
Brooks-Corey	0.15	0.46	0.0452	0.4228
Van Genuchten				
Fixed $m = 1 - 1/n$	0.25	0.46	0.0254	2.3899
Fixed $m = 1 - 2/n$	0.23	0.46	0.0450	2.2528
Silty clay loam (Moderately fine-texture)				
Brooks-Corey	0.25	0.52	0.0321	0.4225
Van Genuchten				
Fixed $m = 1 - 1/n$	0.35	0.52	0.0184	2.4185
Fixed $m = 1 - 2/n$	0.33	0.52	0.0309	2.1910

wide range of pore sizes. They reported λ_{BC} values in the range 0.3 to 10.0 while Szymkiewicz [27] reported that these values generally ranged from 0.2 to 5.0. Zhu and Mohanty [28] 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} equal to 2. Nimmo [29] reported that a medium with many large pores will have a retention function (curve) that drops rapidly to at low soil water content even at low suction head and conversely, a fine-pored medium will retain even at high suction so will have a flatter retention curve. In these functions the hydrodynamic behavior 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. It was also observed (Table 1) that the values of the parameter n decreased as the sand content of these soils increases with constraint $m = 1 - 1/n$ while this trend was observed to be reverse for $m = 1 - 2/n$.

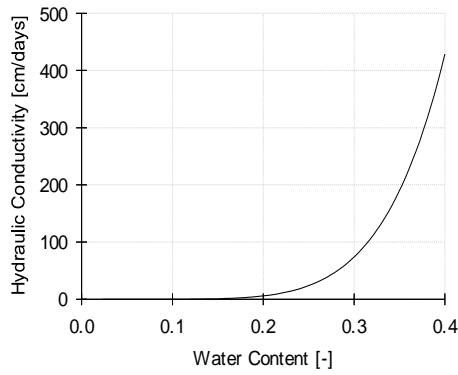
It was observed (Table 2) that the van Genuchten soil water retention function with $m = 1 - 1/n$ gave a slight better fitting in comparison to Brooks-Corey function and van Genuchten function with $m = 1 - 2/n$ for the wet range availability in the sand (coarse texture) soil as the value of r^2 is slightly better for van Genuchten function with $m = 1 - 1/n$ but the RSS values are same for all these functions. For the loam (medium texture) and silty clay loam (moderately fine texture) soils, the best performance was given by the Brooks-Corey function in these soils as indicated by the highest values of r^2 of 0.9973 and 0.9957 in loam and silty clay soils, respectively with least RSS value of 9×10^{-5} for both these soils. Among the van Genuchten function, the better fit was given by the function with $m = 1 - 1/n$ indicated by the corresponding higher r^2 values and lower RSS values for these soils. Mualem [30] reported that there is no single function that fits every soil. Nimmo [31] and Ross et al. [32] also reported that the Brooks-Corey and van Genuchten functions are successful at high and medium water contents but often gave poor results at the low water contents. Mavimbela and van Rensburg [33] also parameterized the soil water retention functions of Brooks-Corey and van Genuchten using RETC code and reported that these functions fitted the measured soil water retention data with r^2 of no less than 0.98.

Table 2. Residual sum of squares (RSS) and coefficient of determination (r^2) of the fitting performance of soil water retention functions

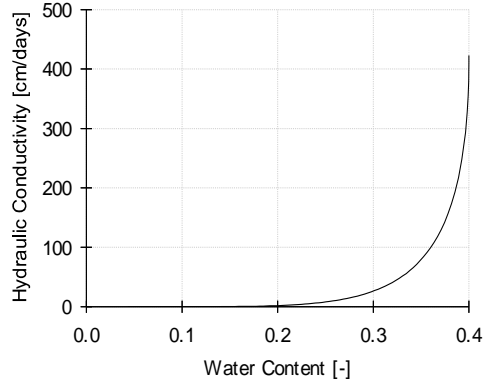
Soil water retention function	Sand (Coarse texture)		Loam (Medium texture)		Silty clay loam (Moderately fine texture)	
	RSS (10^{-5})	r^2	RSS (10^{-5})	r^2	RSS (10^{-5})	r^2
Brooks-Corey	2	0.9997	9	0.9973	9	0.9957
Van Genuchten						
Fixed $m = 1 - 1/n$	2	0.9998	18	0.9951	10	0.9956
Fixed $m = 1 - 2/n$	2	0.9997	37	0.9896	18	0.9916

Mace et al. [34] reported that. The function developed van Genuchten based on the theoretical expression of Mualem predicted hydraulic conductivity more accurately than the van Genuchten function based on the theory of Burdine. So in this study, though both the Burdine and Mualem-based hydrodynamics functions have been evaluated but only the Mualem-based hydrodynamic functions have been shown in the form of graphs considering its preference for accuracy and use. The values of the optimized parameters of these soil water retention functions were used in the corresponding unsaturated hydraulic conductivity and diffusivity functions of Brooks-Corey and van Genuchten for describing the hydrodynamic behavior of these soils. Figs. 1 and 2 depicted the behavior of the hydraulic conductivity and soil water diffusivity functions in relation to soil water content as derived by coupling the Brooks-Corey and van Genuchten functions with Mualem model. It is evident from these Figs.1 and 2 that as the sand content of these soils decreases, the hydraulic conductivity and soil water diffusivity at particular soil water content also decreased. So at specific water content, the hydraulic conductivity and soil water diffusivity were observed to be more in sand and followed by in loam and silty clay loam soils. The hydraulic conductivity and soil water diffusivity based on the coupling of the van Genuchten function with the Mualem model were predicted less in comparison to those predicted by Brook-Corey function when coupled with Mualem model.

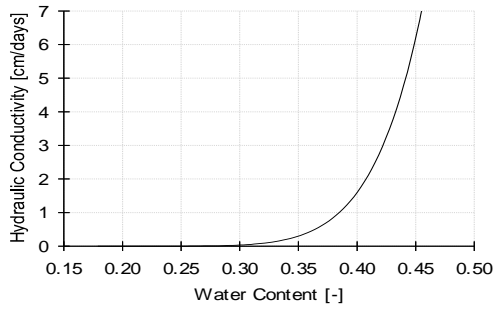
However, general case that for the analytical soil water dynamics, the use of Brooks-Corey function tends to be easier and on the other hand numerical simulation of unsaturated flow, the use of van Genuchten function is mostly adopted.



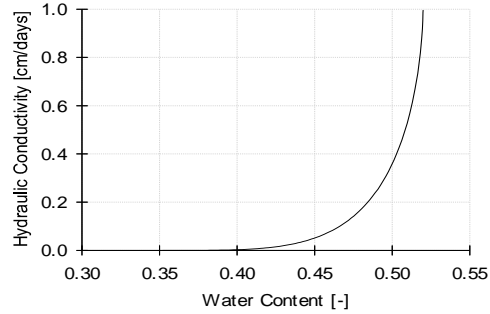
(a)



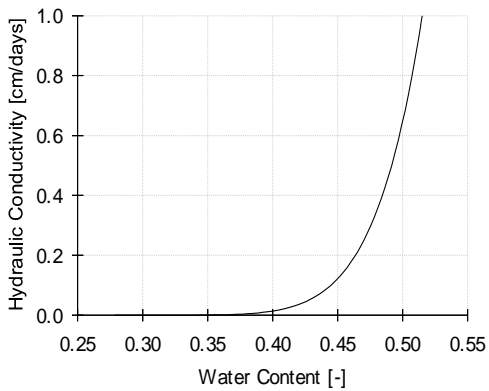
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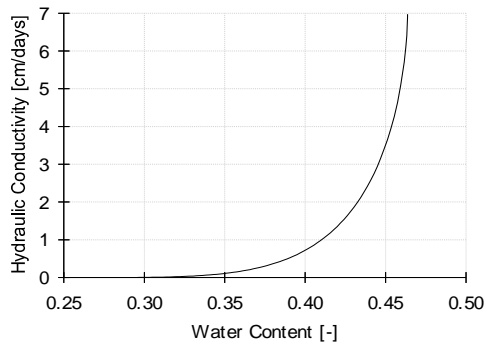
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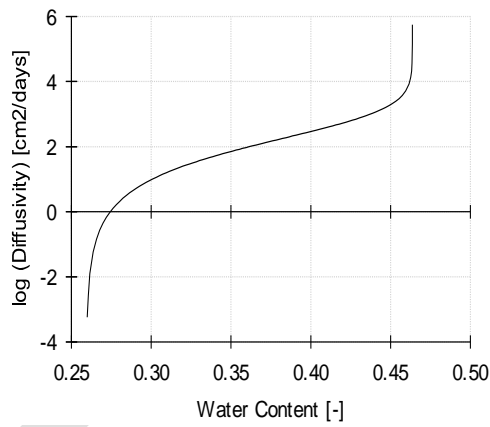
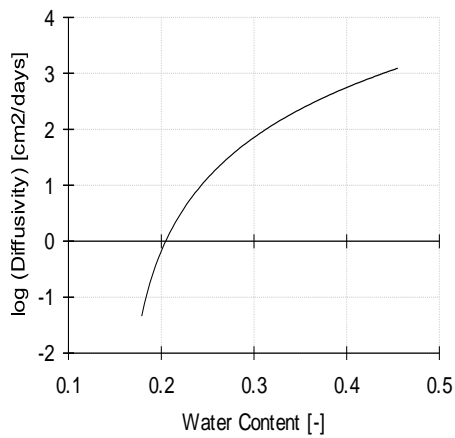
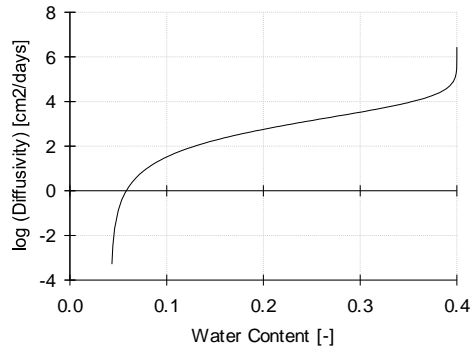
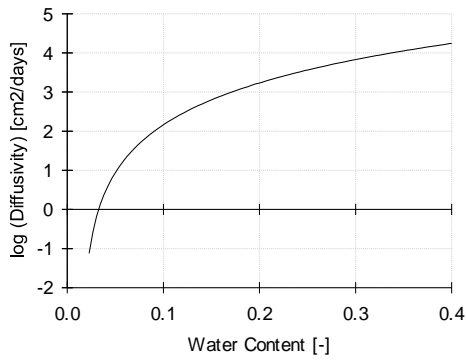


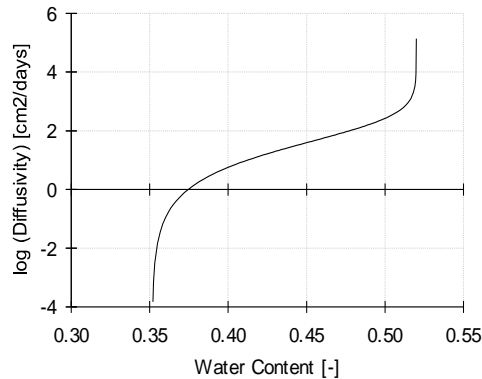
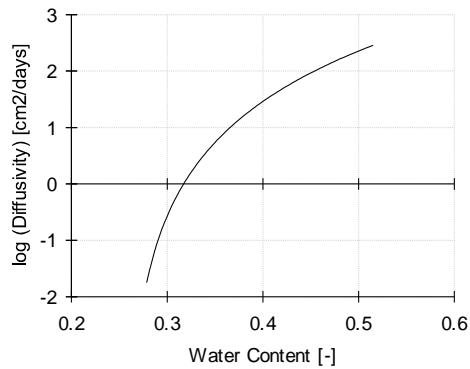
(e)



(f)

Fig. 1. Hydraulic conductivity as a function of water content based on (a) Mualem-Brooks-Corey function for sand, (b) Mualem-van Genuchten function for sand, (c) Mualem-Brooks-Corey function for loam, (d) Mualem-van Genuchten function for loam, (e) Mualem-Brooks-Corey function for silty clay loam, (f) Mualem-van Genuchten function for silty clay loam.





(e)

(f)

Fig. 2. The soil water diffusivity as a function of water content based on (a) Mualem-Brooks-Corey function for sand, (b) Mualem-van Genuchten function for sand, (c) Mualem-Brooks-Corey function for loam, (d) Mualem-van Genuchten function for loam, (e) Mualem-Brooks-Corey function for silty clay loam, (f) Mualem-van Genuchten function for silty clay loam.

Conclusion

For the wet range of water availability in the loam and silty clay loam soil, the best performance was given by the Brooks-Corey soil water retention function followed by van Genuchten functions with $m = 1 - 1/n$ and $m = 1 - 2/n$ but van Genuchten function with $m = 1 - 1/n$ gave slight better performance in sand in comparison to other functions. At a particular soil water content, Mualem-based hydraulic conductivity and soil water diffusivity as predicted by the theoretical by the Brooks-Corey and van Genuchten functions decreased with the decrease in sand content of these soils. The Mualem-van Genuchten function predicted less hydraulic conductivity and water diffusivity in comparison to those predicted by the Mualem-Brooks-Corey function.

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