Simulation of water flow and calculation of the related physical quality indices as influenced by soil water retention curve fitting methods

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Key Points

- The effect of weighting the soil water retention curve data highlighted for particular applications.
- Estimation of soil water retention curve data parameters affected soil physical quality evaluation.
- The simulated water flow in soil was affected by weighting the soil water retention curve data.

Abstract

Accurate fitting of soil water retention curve (SWRC) parameters is crucial in the modeling of soil water flow and the assessment of soil quality. The un-weighted least squares regression (ULS) is the most common approach applied for fitting the SWRC functions to the observed data-points in order to optimize their parameters. However, the variance of SWRC data varies in different water contents; therefore, unlike the wet-end of the SWRC, the ULS method may not be sufficiently effective in estimating its dry-end. This study examined the differences between parameter approximations achieved by the ULS and the weighted least-squares (WLS) in the SWRC. Then, an analysis of both approaches in the simulation of water redistribution and the related soil physical quality indicators (SPQIs) was done. Accordingly, the measured SWRC data in six replications were fitted to the SWRC equations to optimize their parameters, through either WLS or ULS. The results showed that despite the increase of error in the SWRC estimation by the WLS method (*RMSE*=0.027 and 0.043 cm^3 cm^{-3} in the ULS and WLS, respectively), WLS increased the accuracy of the estimations at the lower water contents (dry-end), when compared to the ULS. The WLS regression resulted in different values of SPQIs (e.g., *S*-index = 0.033 and 0.042 or *RFC* (relative field capacity) =

0.57 and 0.62 in the ULS and WLS methods, respectively). Furthermore, the simulated soil water movement in either wet or dry water conditions was different for the SWRC parameter estimated by WLS and ULS regressions.

Keywords: HYDRUS program; Soil physical quality; Soil water flow simulation; Least squares parameter optimization.

1. Introduction

Soil water retention curve (SWRC) parameters are widely used to obtain quantitative information on soil water flow and redistribution, plant water/nutrient uptake, soil and groundwater pollution and salinity, and irrigation (Nakhaei & Šimůnek, 2014), for the purpose of improving agricultural production along with optimizing water consumption (Paredes et al., 2017). Using field/laboratory observational data of SWRC and its parameters is essential for calibrating models before large-scale applications, including the estimation of soil water movement and the solutes transport (Hillel, 1998; Lamorski et al., 2017). Additionally, the SWRCs data can be used to characterize the soil physical quality indicators (SPQIs; Arshad & Martin, 2002), which represent the storage and water/air transmission in soil (Reynolds et al., 2002, 2008). Selected SPQIs driven from SWRC are the air capacity (*AC*), the relative field capacity (*RFC*), the plant available water content (*PAW*), the soil pore size classes, and the so-called *S*-index, which shows the slope of the SWRC at its inflection point (e.g., Topp et al., 1997; Dexter, 2004a; Reynolds et al., 2009, 2014; Zaffar & Sheng-Gao, 2015; Iovino et al. 2016; Koureh et al., 2019). Thus, accurate fitting of SWRCs will lead to the correct calculation of SPQIs. These applications need the description of complete SWRCs using some mathematical function that can best fit the experimental data.

The most common method used to predict the SWRC parameters is fitting a given closed-form SWRC function to the measured datapoints. This means the target absolute error function approaches the constant minima. This is commonly performed through the least-squares (LS) regression in which a particular mathematical SWRC function is fitted to the measured soil water-pressure head, θ (h), data to obtain the SWRC parameters on limited soil samples (van Genuchten et al., 1991). This is typically performed by minimizing the *SSE* (the sum of the squared errors) between the measured and model estimated values of the dependent variable, which is known as the un-weighted LS (ULS) regression (van Genuchten et al., 1991). However, a major shortcoming of this approach is that it implicitly assumes that the data are homoscedastic (i.e., they have constant measurement uncertainty) (Bolster & Tellinghuisen, 2010). However, it is not the case for $\Theta(h)$ data in which the value of the dependent variable (Θ) is decreased with increasing the value of the independent variable (h). Data with heterogeneous measurement uncertainty (i.e., heteroscedastic data) can be better weighted inversely by their variances via the weighted least square (WLS) regression, based on which the minimum-variance estimations of the model parameters and reliable approximations of their standard errors are attained (Draper & Smith, 1998; Seber & Wild, 2003). This results in a more realistic estimate of data error (Tellinghuisen & Bolster, 2009, 2010; Bolster & Tellinghuisen, 2010).

However, this method is mostly considered to address the surface adsorption processes (Cantrell, 2008; Tellinghuisen & Bolster, 2009, 2010; Bolster & Tellinghuisen, 2010). The WLS regression has been revealed to improve parameter estimations and uncertainties, in comparison to the ULS one, in the soil chemical sorption data (e.g., Bolster & Tellinghuisen, 2010), as well as the SWRC data (Sheikhbaglou et al., 2020). In the case of the SWRC data, in the conventional ULS approach, the points close to saturation have a greater contribution to the value of the error function and therefore, SWRC function has a better fit to the wet-end, as compared to the dry-end points. Meanwhile, some processes in the soil (including the redistribution of moisture or transfer of solutes in the soil, especially in the dry and semi-dry conditions) could occur within a small range of SWRC and generally, in the moisture conditions corresponding to the dry end of the SWRC.

As a result, the objective of this study was to examine the differences between parameter approximations achieved by the ULS and the WLS regression in fitting the SWRC function. Subsequently, a functional evaluation was provided using the HYDRUS program to test if the SWRC parameter values adjusted either by the ULS or the WLS regression with different numbers of soil samples could affect the simulation of water redistribution in a given soil. Furthermore, the impact of SWRC fitting methods on the calculation of the related SPQIs was investigated.

2. Materials and methods

2.1. Experimental data

Distributed soil samples were collected from 10 to 30 cm soil depth, and the undisturbed samples were obtained using a cylinder (4.4 cm internal diameter and 5 cm height) from the middle of this depth in six replications (at six points in a 10×10 m^2 plot without vegetation coverage that had been located at the Agricultural Research Site of Urmia University, Iran). In this regard, soil texture, organic matter content, electrical conductivity (EC) and pH were measured by a hydrometer (Dane & Topp, 2002), modified Walkley-Black (Nelson & Somers, 1983), and the saturated extraction of soil (Sparks et al., 2001) methods, respectively. The bulk density of the soil was also determined using undisturbed samples (Blake & Hartge, 1986). The mean soil particle size contained 34.5% clay, 36.5% silt, and 29% sand with a clay loam textural class. Organic matter content, EC, pH, and soil bulk density were 0.8 ± 0.066 %, 0.45 ± 0.006 dS m^{-1}, 8.4 ± 0.076 and 1.38 ± 0.146 g cm^{-3}, respectively. After the saturation of the undistributed soil samples according to Khodaverdiloo et al. (2011), the water content (θ) was measured at 0, 10, 20, 40, 80 and 95 cm pressure heads using the sandbox (the hanging water column method) at 100, 330, 540, 1000, 2000, 4000, 8000 and 15000 cm pressure heads by applying the pressure plates apparatus.

2.2. Determination of the SWRC parameters

2.2.1. Soil water retention curve function

In order to determine the SWRC parameters by the ULS and WLS regression, the SWRC was quantified by van Genuchten (1980) function, using Eq. 1:

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

where θ_s and θ_r are the saturated and residual soil water contents (cm^{3}cm^{-3}), respectively, $S_e(h)$ is the relative saturation (-), h is pressure head (cm), and α (cm^{-1}), m (-) and n (-) are the fitting parameters with m = 1-1/n, according to the Mualem (1976)'s restriction. The van Genuchten model was used for HYDRUS-simulation purposes as it is the most widely used SWRC model (e.g., Patil & Singh, 2016).

2.2.2. Fitting SWRC models to obtain the SWRC parameters

The parameters of van Genuchten (Eq. 1) model were optimized by fitting the model to the measured θ (h) data through the minimization of the sum of the weighted squared errors (SSE; Eq. 2), i.e., the squared differences between observed (θ_m) and model-estimated (θ_p) values of the soil water content:

$$SSE=\sum_{i=1}^{N} w_i(\theta_m-\theta_p)^2 \quad (2)$$

where N stands for the number of measurements and w_i is the i_{th} weighting factor. For the conventional ULS, w_i usually equal to unity for all of the data points; on the other hand, the data were weighted inversely by their variances according to the weighted LS (WLS) regression (Cantrell, 2008; Tellinghuisen & Bolster, 2009, 2010; Bolster & Tellinghuisen, 2010):

$$w_i = \frac{1}{\sigma_{\theta_i}^2} \qquad (3)$$

where $\sigma_{\theta_i}^2$ is the variance of the i_{th} measured water content. In fact, by measuring each point of the SWRC in six replications in this study, the variance of θ (the volumetric soil water content) was calculated at each point and used to calculate the weighting factor.

We used the root mean square error (*RMSE*; Eq. 4), mean error (*ME*; Eq. 5), point error percentage (*EP*; Eq. 6), and the coefficient of determination (R^2; Eq. 7) to evaluate and compare the accuracy of different methods used for fitting the model to the measured SWRC data.

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n} \left(O_i - P_i\right)^2}{n}} \qquad (4)$$

$$ME = \frac{\sum_{i=1}^{n} \left(P_i - O_i\right)}{n} \qquad (5)$$

$$EP = \frac{|O_i - P_i|}{O_i} \times 100 \quad (6)$$

$$R^2 = \left(\frac{\sum (O_i - \overline{O})(P_i - \overline{P})}{\sum (O_i - \overline{O})^2 \sum (P_i - \overline{P})^2} \right)^2 \quad (7)$$

where O_i and P_i are the observed and estimated values, respectively, n is the number of measurements, and p is the number of the model parameters. The *RMSE* index measures the average of the absolute error of the estimates, while *EP* shows the percentage of error at each point and the *ME* index represents the overall overestimation or underestimation of the model. The coefficient of determination is also an indicator of the correlation between the estimated and measured values (Afrasiabi et al., 2019).

The van Genuchten parameters obtained for every soil sample or their mean values over six replications were used to simulate and consequently, to compare the soil water flow (see section 2.4). Two alternative methods were applied to obtain the mean values of the SWRC parameters (Table 1). So, the values of the SWRC parameters obtained for the six soil samples were averaged (method P), or the measured volumetric soil water content of the six soil samples was averaged before fitting the SWRC model to obtain the parameters (method T). This was done to find if taking a single soil sample (as commonly done) or considering either a valid value of SWRC parameters (method P) or an adequate soil sample (method T) could be important in the simulation of the soil water flow and evaluation of the soil physical quality.

The summary of the approaches applied in this study to estimate SWRC parameters is presented in Table 1.

Table 1

2.3. Calculation of the soil physical quality indicators (SPQIs)

2.3.1. Classes of soil pore volume

The cumulative PSD curve was calculated and plotted based on van Genuchten (Eq. 1) SWRC function obtained by both ULS and WLS regressions. According to Kay (1990), three pore size classes based on their equivalent cylinder diameter (i.e., macro- (>30 μm), meso- (0.2-30 μm), and micro-pores (<0.2 μm)), and three pore function classes (i.e., transmission (>50 μm), storage (0.5-50 μm) and residual (<0.5 μm) pores) were calculated, compared and interpreted. In this regard, the equivalent pore diameter, d_E (μm), was determined using the Young-Laplace equation (Or et al., 2002) as:

$$d_E = \frac{4\gamma COS(\omega)}{\rho_W g|h|} \approx \frac{29.74}{|h|}; h<0; d_E(\mu m); 20\,°C \tag{8}$$

where γ=7.28×10^{-2} N m^{-1} is the pore water surface tension, ω is the water-pore contact angle, ρ_w=998.2 kg m^{-3} is water density, and g=9.81 m s^{-2} is the gravitational acceleration.

2.3.2. S index

Dimensionless Dexter's index of soil physical quality, *S*-index (Eq. 9), which represents the slope of the SWRC at the inflection point (Dexter, 2004a, b, c), was calculated using the van Genuchten parameters (Eq. 1) fitted through the ULS and WLS regression (Dexter 2004a):

$$S = -n\left(\frac{\Theta s - \Theta r}{BD}\right)\left[\frac{2n-1}{n-1}\right]^{[1/n-2]}$$

(9)

where BD is bulk density of soil (g cm^{-3}). Larger values of S in soils indicate the abundance of structure pores and better soil physical quality in regard to the root growth of plants, soil tillage and water flow in soil (Dexter, 2004a, b, c).

In this study, the SAWCal calculator software (Asgarzadeh et al., 2014) was used to calculate the S-index based on van Genuchten function parameters.

2.3.3. Air capacity (AC)

AC, indicating the soil aeration condition, could be defined as (Eq. 10):

$$AC = \Theta_S - \Theta_{FC} \tag{10}$$

where Θ_S and Θ_{FC} (equilibrated at h = 330 cm) are the soil water contents (cm^3 cm^{-3}) at the saturation and field capacity, respectively.

2.3.4. Relative field capacity (RFC)

RFC, which indicates the capacity of soil in storing air and water relative to Θ_S, was calculated as shown by (Eq. 11):

$$RFC = \frac{\Theta_{FC}}{\Theta_S} \tag{11}$$

2.3.5. Plant-available water capacity (PAW)

PAW (Eq. 12), which expresses the ability of the soil to store plant-available water, was determined as (Gardner, 1960; Kirkham, 2014):

$$PAW = \Theta_{FC} - \Theta_{PWP} \quad (12)$$

where Θ_{PWP} is the ‘‘permanent wilting point’’ soil water content (cm^3 cm^{-3}) equilibrated at 15000 cm pressure head.

2.4. Simulation of the water flow in soil

In order to investigate if the differences in the SWRC parameters estimated through ULS and WLS regression and the way applied to average their values could functionally affect soil water flow simulations, a simple two-dimensional soil water flow project was simulated in the HYDRUS program. In this project, surface drip irrigation in a uniform soil with the depth and width of 1 m (dripper in the middle of the soil surface) was considered. Irrigation was carried out for 12 hours with the discharge of 0.5 l h^{-1}, and simulation was performed for a week with a constant value of potential evaporation from the soil surface (cm day^{-1}). Initial volumetric soil water conditions were defined as the normal amounts of 25%. A time-variable flux boundary condition was applied at the center of the soil surface to represent the drip irrigation, which was switched to the atmospheric boundary condition during the period with no irrigation. The atmospheric and free drainage boundary conditions were considered on the remainder of the soil surface and the bottom of the soil profile, respectively. No flux boundary condition was applied on the left and right sides of the soil profile. The simulation domain and the selected boundary conditions are shown in Fig. 1.

The SWRC parameters obtained with different methods, which have been described in Table 1, were considered in the simulations of soil water flow. Also, the saturated hydraulic conductivity of the soil was estimated in the field based on the BEST-steady method (Bagarello et al., 2014).

Fig. 1

3. Results and discussion

3.1. The effect of weighting the SWRC data on the model fit and SWRC parameters

A statistical description of the measured SWRC data is presented in Table 2. The coefficient of the variation of the measured soil water contents was gradually increased with raising the pressure heads (Table 2). This was most likely due to the unreliability of the pressure plates apparatus used to determine the SWRC in the dry-end, the lack of the soil–plate contact, no hydrostatic equilibrium, soil dispersion, and low plate and soil conductance (Campbell, 1988; Gee et al., 2002; Solone et al., 2012). The weighting factors of the WLS regression were calculated as the inverse of variances at each pressure head (Fig. 2). The weighting factors were lower at the higher water contents; so they were higher at the dry-end (higher pressure heads) too (Fig. 2), due to the lower standard deviation of the measured soil water contents at the higher pressure heads (Table 2). By considering these weighting factors, the van Genuchten SWRC parameters were obtained using WLS and compared with those obtained by the ULS regression (Table 3). The values of the obtained SWRC parameters differed considerably in WLS and ULS (Table 3). So, the values of the residual water content (θ_r), saturation water content (θ_s) and α parameters were lower in the WLS, as compared to those in the ULS regression. On the other hand, the *n* parameter had higher values in the WLS regression. These differences may practically lead to various SWRCs and SPQIs, resulting in different estimates of the soil behaviour, including the distribution of water and the solutes transport in the soil.

Table 2

Fig. 2

Table 3

The values of R^2 for the van Genuchten model were higher in the ULS (from 0.89 to 0.94), as compared to those obtained by the WLS regression (ranged from 0.81 to 0.91). Although the WLS regression generally resulted in an increase of error in estimating the SWRC and a reduced correlation between the estimated and observed water contents (Table 4), it improved the accuracy of the estimations at the lower water contents (Fig. 3). The practical relevance of these results is for some processes governing such soil behaviours as water redistribution and contaminant transport; this is especially the case in arid and semi-arid conditions in which they occur at lower soil water contents, thus corresponding to the dry-end of the SWRC. Since, in the conventional ULS method, data points closer to the saturation have a more significant contribution to the optimization objective function (i.e., *SSE*), the SWRC model is forced to be fitted to the wet-end rather than the dry-end. Meanwhile, assigning appropriate weights to the SWRC data could improve the fit of the SWRC model to its dry-end. In the previous studies on chemical sorption processes by Cantrell (2008), Tellinghuisen and Bolster (2009, 2010) and Bolster and Tellinghuisen (2010), the use of the WLS regression and assignment of appropriate weights in fitting the governing models have been emphasized. The *ME* values in the WLS-fitted van Genuchten model were negative for all samples (Table 4), indicating the underestimation of the soil water content by the model. In contrast, the ULS-fitted van Genuchten model did not show any considerable under/over-estimation.

Table 4

Fig. 3

Owing to the high spatial variability of soil physical and hydraulic properties (e.g., Schaap et al., 2001), it may be crucial to perform different replications in the quantification of the SWRC for practical applications, rather than using a single soil sample data, as usually done. Consequently, two averaging alternatives were compared to obtain the SWRC parameters (Table 5) and to quantify the studied SPQIs (Table 6). Two averaging methods were used, namely, P (averaging the values of SWRC parameters obtained for replicative soil samples through a given fitting process (i.e., ULS or WLS regression) and T (averaging the values of the volumetric soil water content measured at each of the pressure heads for the replications to obtain a "mean-soil" SWRC data and to estimate the SWRC parameters) methods (see Table 1). The SWRCs calculated by the van Genuchten model parameters that had been obtained with these two averaging methods (see Table 5) were compared to the observations (Fig. 4a). In general, the T method provided more accurate estimates of the SWRC than the P one for the van Genuchten model (Table 5).

Similar to the single soil sample data, the two averaged WLS-fitted van Genuchten models provided more accurate estimate at the lower water contents (Fig. 4a). However, as expected, the averaged ULS-fitted van Genuchten model estimates were more accurate at the wet-end of SWRCs (Figs. 4a). Therefore, if one evaluates the model in terms of its general performance for describing the entire SWRC, the ULS-fitted model is more accurate. In contrast, the WLS-fitted model performs better in estimating the dry-end, which is practically vital for such conditions as water redistribution in relatively dry soils. Similarly, Afrasiabi et al. (2019), in evaluating the selected particle size distribution models, concluded that a specified model might be well accurate, generally in terms of producing the entire particle size distribution curve; however, locally, it fails to estimate the selected parameters or particular points of the curve.

Table 5

Fig. 4.

3.2. The effect of weighting the SWRC data on the interpretation of the soil physical quality

Pore size distribution (PSD) curves based on van Genuchten SWRC parameter values that had been obtained through ULS and WLS regression by following the applied averaging schemes are shown in Fig. 4b. Pore size and functional classes are also presented in Fig. 5. Considerable dissimilarities were detected between WLS- and ULS-fitted van Genuchten parameters in calculating the soil PSD (Figs. 4b and 5). However, the averaging schemes showed no significant differences in this regard.

Fig. 5

Soil physical quality indices calculated with the SWRC parameters that had been obtained through ULS and WLS regression are compared in Table 6. The WLS regression resulted in the higher values of the *S*-index, as compared to the ULS one. The mean value of the *S*-index was calculated based on WLS-fitted SWRC parameters, which was 0.041, while it was 0.030 for the ULS regression (Table 6). It was also the same for the averaging schemes applied to the WLS and ULS regression estimates (Table 6). The *S*-index commonly depends on soil microporosity, that is strongly influenced by management practices (Dexter, 2004a); the higher the S value, the greater the intensity of available water and better the conditions for the root and plant growth. The theoretical limits of the *S*-index are $0 \leq S < \infty$; however, practically, the following categories have been suggested: $S \geq 0.050$: perfect soil physical or structural quality, $0.050 > S \geq 0.035$: good physical quality, $0.035 > S \geq 0.020$: poor physical quality, and $0.020 > S$: very poor or degraded physical quality (Dexter 2004a, b, c; Dexter & Czyz, 2007; Tormena et al., 2008). Therefore, according to the WLS-fitted SWRC parameter values, the studied soils had *S*-index values in the range of 0.035 to 0.050; so, they had a "good" physical quality. However, they showed a "poor" physical quality based on the ULS-fitted parameters. As seen, the weighing of the SWRC data could affect the interpretation one may make regarding the soil physical quality.

The ULS regression resulted in the higher mean values of all other SPQIs, except for *PAW* and *RFC,* for which the WLS regression provided higher mean values (Table 6). However, these differences do not make any sense from a practical point of view. An $AC \geq 0.10$ m^{3}m^{-3} has conventionally been suggested in terms of soil physical limitations for the minimum susceptibility to plant-damaging or yield-reducing aeration deficits in the root zone (White, 2006); however, more recent works have exhibited that $AC \geq 0.14$ m^{3}m^{-3} is required in the soils with sandy loam or clay loam textures for optimal aeration (Carter, 1988; Drewry, 2006; White, 2006; Mueller et al., 2009). On the other hand, *RFC*, which expresses the soil's ability to store water and air, relative to the total porosity, is supposed to be optimal when $0.6 \leq RFC \leq 0.7$, providing desirable water and air contents for the plant growth (Doran et al., 1990; Olness et al., 1998; Reynolds et al., 2002). The lower values of *RFC* (i.e., $RFC < 0.6$) cause insufficient soil water, while the greater ones ($RFC > 0.7$) result in the insufficient soil air (i.e., "aeration limited" soil) (Linn & Doran, 1984; Doran et al., 1990; Skopp et al., 1990; Olness et al., 1998; Reynolds et al., 2003). *PAW* indicates the ability of the soil to store water and make it available for plant use (Kirkham, 2014). Therefore, a high *PAW* is indicative of the good soil physical quality. Plant growth is enhanced with increasing *PAW* (Dörner et al. 2013; Descalzi et al. 2018). Hall et al. (1977), Warrick (2001) and White (2006) have suggested the following categories for *PAW*: $0.20 > PAW \geq 0.15$ cm^3 cm^{-3}: good, $0.15 > PAW \geq 0.10$ cm^3 cm^{-3}: medium or limited, and $PAW < 0.10$ cm^3 cm^{-3}: poor or droughty. Furthermore, $PAW \geq 0.20$ m^3 m^{-3} has been introduced as the ideal for the maximal root growth and function (Hall et al., 1977).

Different soil sample measurements (i.e., replications) resulted in different values of SPQIs (Table 6), including the *S*-index (ULS: 0.023-0.034; WLS: 0.034-0.044), *PAW* (ULS: 0.08-0.13; WLS: 0.12-0.19), *AC* (ULS: 0.08-0.23; WLS: 0.06-0.22) and *RFC* (both ULS and WLS: 0.5-8). According to the above-mentioned limits and categories, one can see that these differences lead to opposite interpretations regarding the soil physical quality. Therefore, it is of practical relevance not to make management decisions based on some single soil sample measurements.

Table 6

3.3. The effect of weighting the SWRC data on soil water distribution simulations

In order to investigate the weighting effect of the SWRC data on soil water flow simulation, the spatial and temporal variations of the soil water content were simulated. Fig. 6 shows the water advance front shape in the soil profile in both WLS and ULS regressions for two representative soil samples (as examples) and two averaging methods applied. The weighting effect on different SWRC parameters of soil (as shown in Tables 3 and 5) affected the simulation results of water movement in the soil; so, WLS and ULS provided different soil water advance front profiles (Fig. 6). In this way, the water advance front shape in the ULS method is moistened vertically. On the other hand, in the case of the WLS method, water entering the soil is distributed in all directions. Using different soil samples also resulted in different simulations of the soil water movement (compare S2 and S5 simulations in Figs. 6 and 7).

Furthermore, soil water content changes over time (one-week simulation duration) at a specific point in the soil profile (at the soil surface in the vicinity of the emitter) for two representative soil samples (as examples), as well as for the two averaging methods applied, were compared for WLS and ULS methods (Fig. 7). The duration of the simulation was continued until the soil water content reached from relatively wet conditions to relatively dry water ones in order to investigate the effect of weighting on the simulation of water flow in soil under different water conditions. As shown in Fig. 7, the weights caused the soil water content in the wet range (from saturation to almost field capacity condition) to be less than that in the ULS; in contrast, in the dry range (from the field capacity to lower water contents), it was more than that in the ULS. The simulation results, therefore, showed that the weighting of the SWRC data had a significant effect on the soil water flow simulation in two wet and dry water conditions. However, the differences between the used averaging methods were not considerable.

Fig. 6

Fig. 7

3.4. Possible limitations and implications of the investigation

In this research, the un-weighted and weighted least-squares fitting process of SWRC and their impact on the simulations of soil water flow and the related soil physical quality indicators (SPQIs) were evaluated. The results were based on some experiments. The specific possible errors and limitations included preparation of the undistributed soil samples to measure the SWRC, as well as possible errors related to the SWRC measurement with sandbox and the pressure plates apparatus used to measure the equilibrium time. Furthermore, these results were obtained for a specific soil texture to highlight this issue. Therefore, we acknowledge that the results obtained in this study are not sufficient to draw strong conclusions. Consequently, a similar analysis in different soil textures and conditions, comparison of the simulation results with the measured data, consideration of different scenarios of water flow in soil for simulation (such as those under the impact of root water uptake and with real values of soil surface evaporation), investigation other bimodal hydraulic functions and also, other dispersion scenarios, especially at lower pressure heads, need to be evaluated in the future studies to reach more definite conclusions.

4. Conclusion

Weighting the soil water retention curve (SWRC) data based on the least square analysis led to obtaining some values for the SWRC parameters that were different from those estimated by the conventional un-weighted least-squares (ULS) regression. Although the ULS regression generally resulted in the better fitting of the SWRC model, the weighted least-squares (WLS) regression increased the accuracy of the estimations at lower water contents, which could be of practical relevance when such soil behaviours as water redistribution need to be estimated at lower soil water contents. The results suggested that using the WLS regression and assigning appropriate weights in fitting the SWRC model need to be emphasized for particular applications. The results also suggested that it would be crucial to perform different replications in the quantification of the SWRC for practical applications, rather than using a single soil sample data, as usually done. As the conclusion, a specified SWRC model may well be accurate, generally in terms of producing the entire SWRC, while failing locally to estimate the soil water content at some specific (and practically relevant) pressure head. Furthermore, the weighing of the SWRC data could affect the calculated values of the studied soil physical quality indicators, resulting in interpretations different from those made based on the ULS-fitted parameters. The results also showed that the weighting of the SWRC data had a significant effect on water flow simulation in the soils with contrasting water conditions.

Data Availability Statement

Experimental data for soil water retention curve and simulation results for soil water flow are available in an archived Zenodo repository (https://zenodo.org/record/4316621).

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Table 1. Summary of the methods used for estimating the soil water retention curve (SWRC) parameters

Method	Methods used for determining the SWRC parameters
ULS	The method of fitting the van Genuchten SWRC function to the measured SWRC data of a single soil sample (S1-S6) by using the conventional un-weighted least squares (ULS) regression to obtain the SWRC parameters.
WLS	The method of fitting the van Genuchten SWRC function to the measured SWRC data of a single soil sample (S1-S6) by using the weighted least squares (WLS) regression to obtain the SWRC parameters.
T-ULS	Measuring the SWRC in a specified number of replications (six replicated

	soil samples in this study), averaging the water contents at each pressure head, and fitting the SWRC function by using the conventional ULS regression to obtain the SWRC parameters.
P-ULS	Measuring the SWRC in a specified number of replications (six replicated soil samples in this study), fitting the SWRC function using the conventional ULS regression to obtain the SWRC parameters for each soil sample, and averaging the parameters values on the replications.
T-WLS	Measuring the SWRC in a specified number of replications (six replicated soil samples in this study), averaging the water contents at each pressure head, and fitting the SWRC function using the WLS regression to obtain the SWRC parameters.
P-WLS	Measuring the SWRC in a specified number of replications (six replicated soil samples in this study), fitting the SWRC function using the WLS regression to obtain the SWRC parameters for each soil sample, and averaging the parameters values on the replications.

Table 2. Statistical parameters of the measured volumetric soil water content ($cm^3\ cm^{-3}$) at different pressure heads for the six replicates

Table 3. Soil water retention curve parameters obtained via weighted (WLS) and un-weighted least-squares (ULS) fitting of the van Genuchten model

Fitting method	Soil sample	van Genuchten parameters			
		Θ_r ($cm^3\ cm^{-3}$)	Θ_s ($cm^3\ cm^{-3}$)	α (cm^{-1})	n (-)
ULS	S1	0.015	0.452	0.192	1.16
	S2	0.000	0.362	0.011	1.16
	S3	0.000	0.431	0.189	1.16
	S4	0.001	0.467	0.210	1.14
	S5	0.000	0.462	0.333	1.15
	S6	0.000	0.419	0.424	1.11
	Mean	0.000	0.432	0.227	1.15
	C.V. (%)	223.61	9.02	62.33	1.71
WLS	S1	0.001	0.431	0.050	1.23
	S2	0.001	0.358	0.004	1.31
	S3	0.001	0.404	0.037	1.26
	S4	0.000	0.439	0.040	1.23
	S5	0.001	0.436	0.066	1.22
	S6	0.000	0.374	0.024	1.22
	Mean	0.001	0.407	0.037	1.25
	C.V. (%)	77.46	8.47	57.93	2.82

C.V.: Coefficient of variations

Table 4. Statistical criteria for the evaluation and comparison of weighted (WLS) and un-weighted least-squares (ULS) fitting of the studied soil water retention curve function in predicting the volumetric soil water content

Fitting Method	Soil sample	*RMSE* (cm^3 cm^{-3})	*ME* (cm^3 cm^{-3})	R^2
ULS	S1	0.024	-0.000	0.934
	S2	0.024	0.001	0.894
	S3	0.023	0.000	0.938
	S4	0.027	0.000	0.923
	S5	0.023	-0.000	0.939
	S6	0.024	0.000	0.901
	Mean	0.024	0.000	0.922
	C.V. (%)	6.09	244.95	2.12
WLS	S1	0.035	-0.010	0.907
	S2	0.034	-0.008	0.881
	S3	0.037	-0.013	0.900
	S4	0.041	-0.012	0.883
	S5	0.036	-0.011	0.904
	S6	0.042	-0.012	0.815
	Mean	0.038	-0.011	0.882
	C.V. (%)	8.72	-16.26	3.90

C.V.: Coefficient of variations

Table 5- Soil water retention curve (SWRC) parameters and statistical evaluation indices in estimating the SWRC in weighted- and unweighted-least squares regression (WLS and ULS) and the averaging methods applied (P and T) (see Table 1 for the details)

	Method	Θ_r (cm^3 cm^{-3})	Θ_s (cm^3 cm^{-3})	α (cm^{-1})	n (-)
SWRC parameters	P-ULS	0.0028	0.432	0.226	1.15
	P-WLS	0.0006	0.407	0.0369	1.25
	T-ULS	0.0007	0.433	0.197	1.14
	T-WLS	0.0006	0.402	0.0285	1.24
	Method	*RMSE* (cm^3 cm^{-3})	*ME* (cm^3 cm^{-3})	R^2	
Statistical evaluation indices	P-ULS	0.0266	-0.012	0.927	
	P-WLS	0.0432	-0.021	0.890	
	T-ULS	0.0234	0.000	0.928	
	T-WLS	0.0389	-0.012	0.878	

Table 6-Comparision of soil physical quality indicators in weighted- and unweighted-least squares regression (WLS and ULS) and the averaging methods applied (P and T) (see Table 1 for the details)

Method	Θ_S (cm^3 cm^{-3})	Θ_{FC} (cm^3 cm^{-3})	Θ_{PWP} (cm^3 cm^{-3})	*S*-Index (-)	*AC* (cm^3 cm^{-3})	*RFC* (-)	*PAW* (330) (cm^3 cm^{-3})
S1-ULS	0.451	0.239	0.137	0.033	0.212	0.530	0.102
S2-ULS	0.362	0.285	0.156	0.024	0.077	0.787	0.128
S3-ULS	0.431	0.226	0.125	0.032	0.205	0.525	0.101

S4-ULS	0.467	0.253	0.146	0.033	0.214	0.541	0.107
S5-ULS	0.462	0.233	0.133	0.034	0.230	0.503	0.099
S6-ULS	0.419	0.240	0.156	0.023	0.179	0.573	0.084
Mean	0.432	0.246	0.142	0.030	0.186	0.577	0.104
C.V. (%)	9.00	8.57	8.91	16.61	30.09	18.32	13.81
S1-WLS	0.431	0.227	0.097	0.042	0.204	0.527	0.130
S2-WLS	0.358	0.295	0.104	0.038	0.063	0.825	0.191
S3-WLS	0.404	0.211	0.080	0.044	0.193	0.522	0.131
S4-WLS	0.439	0.238	0.098	0.044	0.201	0.543	0.140
S5-WLS	0.436	0.217	0.093	0.044	0.219	0.498	0.124
S6-WLS	0.374	0.232	0.101	0.034	0.142	0.621	0.132
Mean	0.407	0.237	0.096	0.041	0.170	0.589	0.141
C.V. (%)	8.47	12.77	8.85	10.12	34.51	20.84	17.59
P-ULS	0.432	0.230	0.132	0.030	0.202	0.532	0.098
T-ULS	0.433	0.244	0.145	0.029	0.189	0.563	0.099
P-WLS	0.407	0.219	0.086	0.041	0.189	0.537	0.130
T-WLS	0.402	0.234	0.096	0.040	0.169	0.580	0.138

C.V.: Coefficient of variations

FIGURES CAPTIONS:

Fig. 1. Conceptual geometry and boundary conditions in the HYDRUS (2D/3D) simulations.

Fig. 2. Calculated weights for the weighted-least squares regression at different pressure heads.

Fig. 3. Comparison of the observed soil water retention curves with those calculated using the soil water retention curve parameters obtained via weighted- and unweighted-least squares regression (WLS and ULS) for two representative soil samples (S2 and S5) in the van Genuchten function.

Fig. 4. Comparison of the observed soil water retention curves with those calculated using the soil water retention curve parameters obtained via weighted- and unweighted-least squares regression (WLS and ULS) and the averaging methods applied (P and T) in the van Genuchten model (a) and calculated cumulative pore size distribution curves (b).

Fig. 5. Comparison of the pore fractions in different sizes based on van Genuchten soil water retention curve function in weighted- and unweighted-least squares regression (WLS and ULS) and the averaging methods applied (P and T).

Fig. 6. Simulation of water flow in the soil profile in weighted- and unweighted-least squares regression (WLS and ULS) in two representative soil samples (S2 and S5) and the averaging methods applied (P and T).

Fig. 7. Comparison of the simulated temporal variation of the soil water content in the soil surface near the dripper in weighted- and unweighted-least squares regression (WLS and ULS) in two representative soil samples (S2 and S5) and the averaging methods applied (P and T).

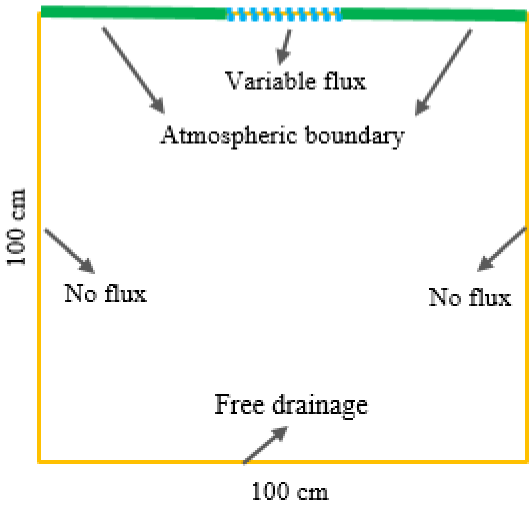


Fig. 1.

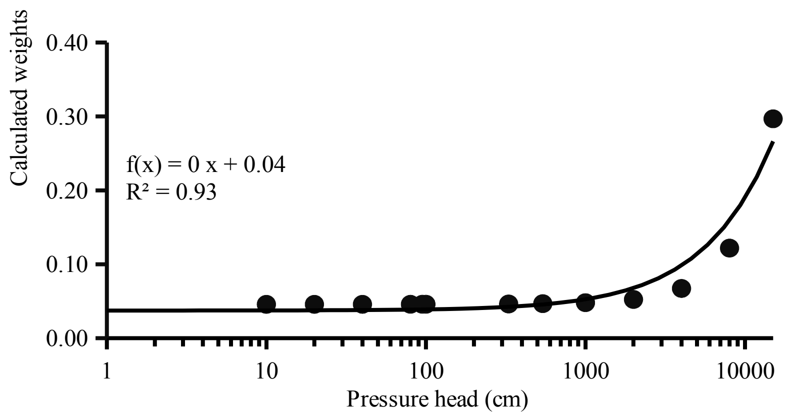


Fig. 2.

S2 S5

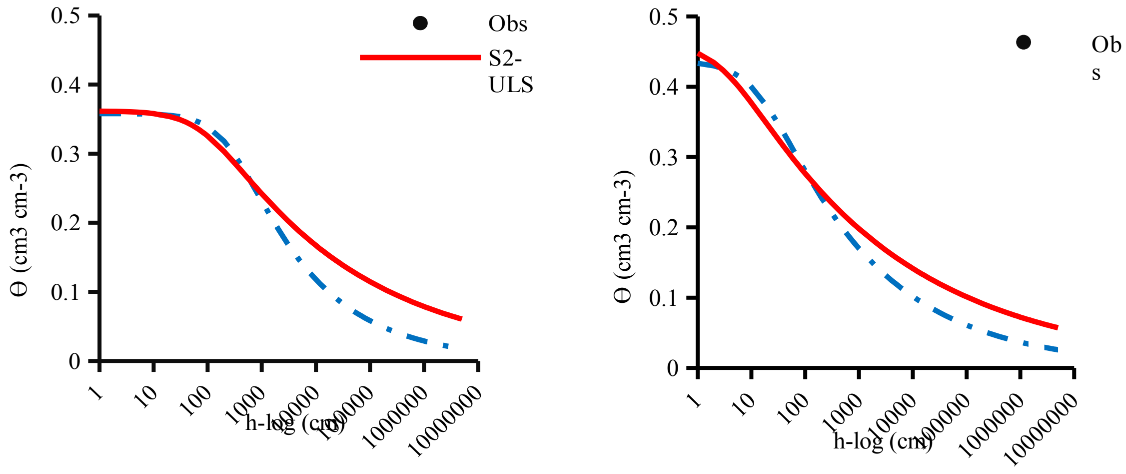


Fig. 3.

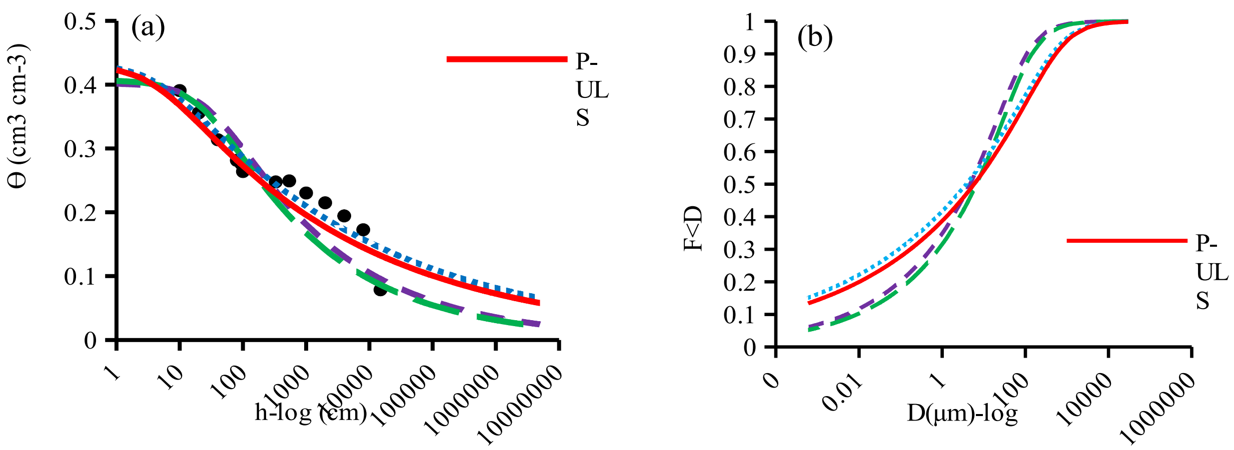


Fig. 4.

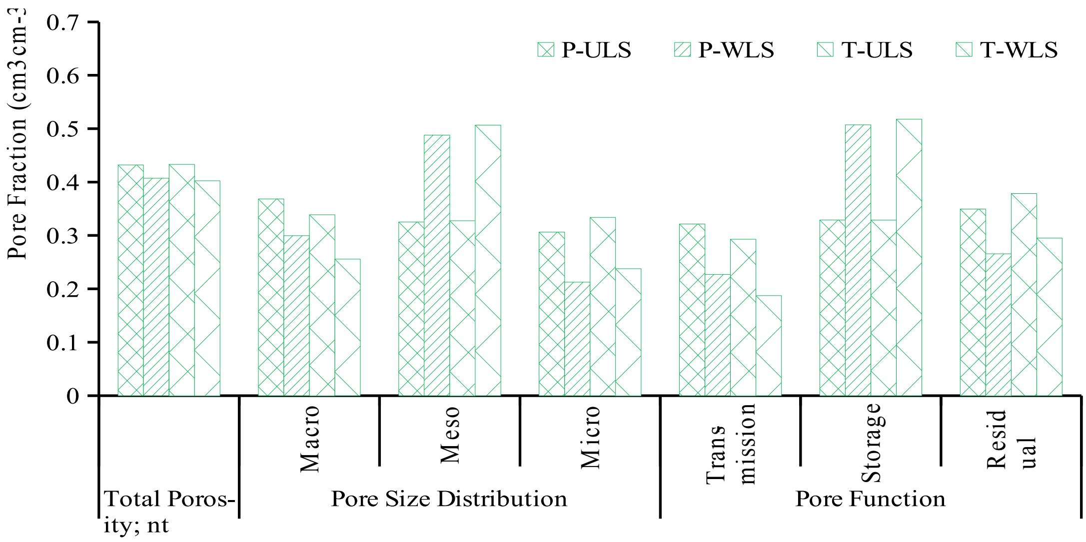


Fig. 5.

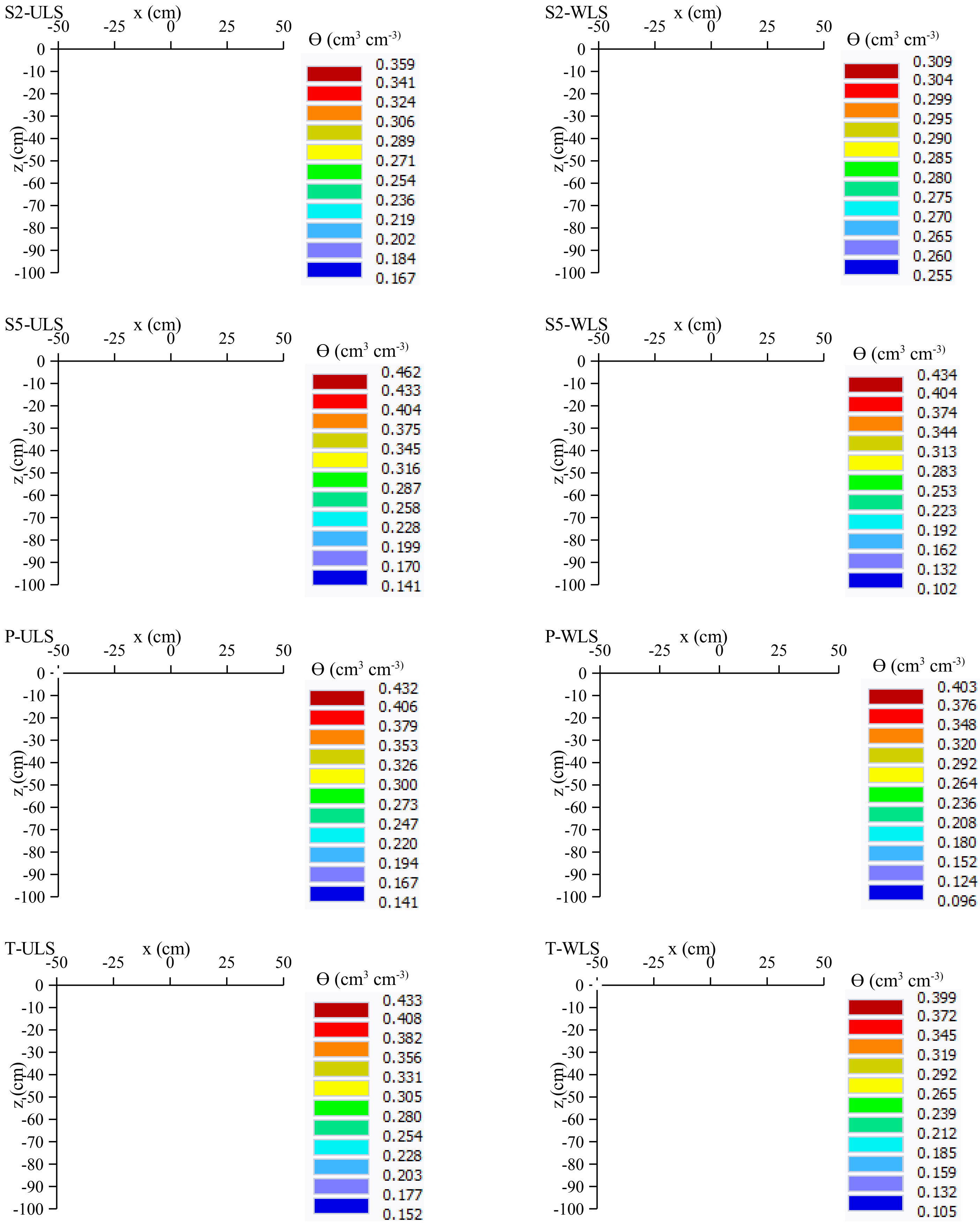
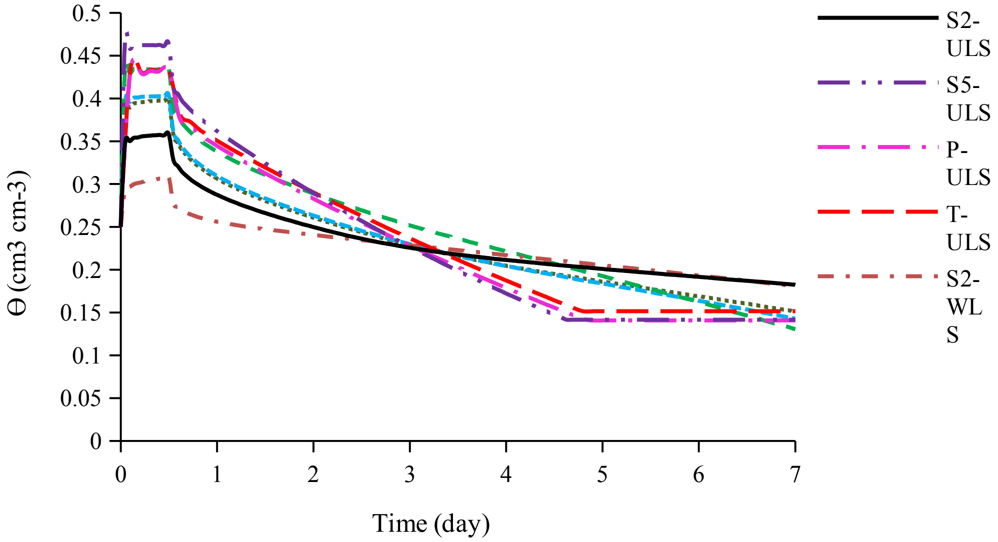

S2-ULS
x (cm)
-50 -25 0 25 50
z (cm)
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100
Θ (cm³ cm⁻³)
0.359 0.341 0.324 0.306 0.289 0.271 0.254 0.236 0.219 0.202 0.184 0.167
S2-WLS
x (cm)
z (cm)
Θ (cm³ cm⁻³)
0.309 0.304 0.299 0.295 0.290 0.285 0.280 0.275 0.270 0.265 0.260 0.255
S5-ULS
x (cm)
z (cm)
Θ (cm³ cm⁻³)
0.462 0.433 0.404 0.375 0.345 0.316 0.287 0.258 0.228 0.199 0.170 0.141
S5-WLS
x (cm)
z (cm)
Θ (cm³ cm⁻³)
0.434 0.404 0.374 0.344 0.313 0.283 0.253 0.223 0.192 0.162 0.132 0.102
P-ULS
x (cm)
z (cm)
Θ (cm³ cm⁻³)
0.432 0.406 0.379 0.353 0.326 0.300 0.273 0.247 0.220 0.194 0.167 0.141
P-WLS
x (cm)
z (cm)
Θ (cm³ cm⁻³)
0.403 0.376 0.348 0.320 0.292 0.264 0.236 0.208 0.180 0.152 0.124 0.096
T-ULS
x (cm)
z (cm)
Θ (cm³ cm⁻³)
0.433 0.408 0.382 0.356 0.331 0.305 0.280 0.254 0.228 0.203 0.177 0.152
T-WLS
x (cm)
z (cm)
Θ (cm³ cm⁻³)
0.399 0.372 0.345 0.319 0.292 0.265 0.239 0.212 0.185 0.159 0.132 0.105

Fig. 6.



0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
0 1 2 3 4 5 6 7
Θ (cm3 cm-3)
Time (day)
S2-
ULS
S5-
ULS
P-
ULS
T-
ULS
S2-
WL
S

Fig. 7.