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Estimation of van Genuchten Equation Parameters in Laboratory and through Inverse Modeling with Hydrus-1D

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Abstract

Soil water retention curve (SWRC) becomes important because it guides when and how much to irrigate, optimizing the use of water; can be obtained in the field or laboratory, being commonly determined in the laboratory with porous plate apparatus, and the determination is compromised by issues such as time and labor. In this context, inverse modeling emerges, which allows to obtain a variable going from the effect to the cause, using Hydrus-1D. Hence, this study aims to obtain van Genuchten equation parameters through inverse modeling with Hydrus-1D and make the respective comparisons and inferences. Matric potential data were obtained over time in an instantaneous profile-type experiment. Six sets of three tensiometers each were installed surrounding the center of the experimental plot, at depths of 0.20, 0.35 and 0.50 m. Target depth was 0.35 m, where the roots of most crops are concentrated, and the other tensiometers were used to obtain the potential gradient. Matric potential data were used to feed Hydrus-1D and obtain the van Genuchten equation parameters. Laboratory curves were obtained using porous plate apparatus, with four replicates. It was concluded that, in general, the Hydrus-1D model estimates van Genuchten equation parameters and, consequently, the SWCC of an Argissolo more consistently with field conditions than those obtained in the laboratory; and, provided it is fed with field data, the Hydrus-1D simulates well the behavior of matric potential and moisture over time, reducing the time and labor in the procedures to obtain van Genuchten equation parameters in the laboratory.

Keywords: instantaneous profile, methodology in soil, soil-water characteristic curve

1. Introduction

Knowledge on soil physical attributes, like hydraulic properties, is important for the agricultural sustainability, guiding strategies that lead to maximum crop yield (Imhoff et al., 2016). In this context, the soil water retention curve (SWRC), given by the relationship between water content and the matric potential with which water is retained in the soil—allows to monitor soil moisture and, therefore, define when and how much to irrigate (Lucas et al., 2011).

SWRC can be obtained through various methods, in the field and laboratory. However, it is usually determined under laboratory conditions using the porous plate apparatus, proposed by Richards and Fireman (1943), in which the water content retained in the sample under the applied pressure originates the curve (Menezes et al., 2018). SWRC shape is commonly described by an empirical equation and the model of van Genuchten (1980), with five parameters, is the most used for this purpose, because it fits to a wide variety of soils (Xiang-Wei et al., 2010).

Obtaining soil hydraulic parameters, such as SWRC, either in the field or laboratory, is often demanding, in both time and labor, which makes such determination unviable in some cases (Singh et al., 2010). In this context, inverse modeling emerges, which is nothing more than obtaining certain variable through the solution of an inverse mathematical problem. In other words, it is possible to mathematically obtaining unmeasurable parameters of a system from mensurable ones since they have a physical relationship (Hasanoğlu & Romanov, 2017).

The Hydrus-1D model, whose 4.17 version is signed by Šimůnek et al. (2013), is widely used to obtain soil hydraulic parameters, such as hydraulic conductivity and variables of the van Genuchten model, based on inverse problems. The user must enter the evolution of soil moisture or matric potential over time as input data, which are the basis for the simulation.

Given the above, this study considered the hypothesis that the Hydrus-1D model, for being based on physical processes, simulates van Genuchten equation parameters and, consequently, the SWRC of an Argissolo more consistently with the field conditions than those obtained in the laboratory, besides reducing the time and labor of the procedure. Hence, this study aimed to obtain van Genuchten equation parameters of an Argissolo through inverse problem using Hydrus-1D and in the laboratory, and make the respective comparisons and inferences.

2. Material and Methods

2.1 Field and Laboratory Work

Field work was carried out in a Argissolo Amarelo (EMBRAPA, 2013), where an instantaneous profile experiment was installed, specifically at UTM coordinates 9586090 N and 546494 L (Figure 1). Instantaneous profile experiment was selected because this test allows to monitor the variation of soil water matric potential during the drainage process, a parameter that served as basis for the inverse modeling using Hydrus-1D, described hereinafter.

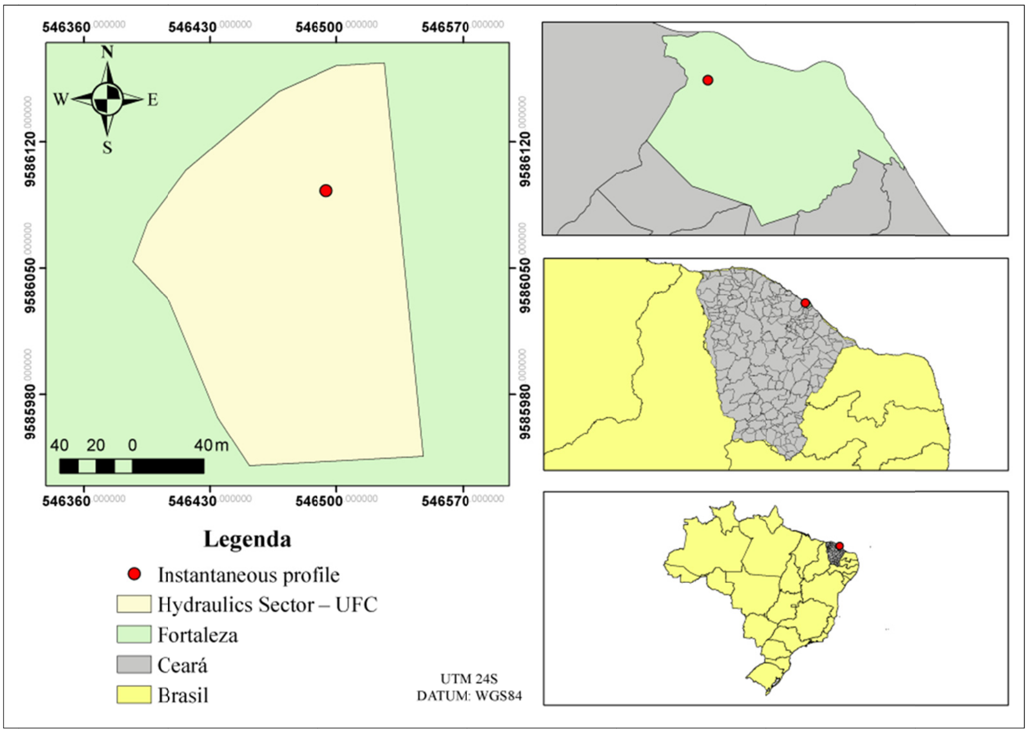

Figure 1. Instantaneous profile Hydraulics Sector—UFC (Fortaleza, Ceará, Brazil)

The instantaneous profile-type experiment followed the methodology proposed by Hillel et al. (1972) and was carried out in a circular plot with diameter of 3.0 m and depth of 0.60 m. The experimental plot was delimited by a plastic canvas to allow vertical water flow. Six sets with three tensiometers each were installed surrounding the center of the experimental plot, at depths of 0.20, 0.35 and 0.50 m. Target depth in the present study was 0.35 m, the effective depth of the root system of most cultivated species. The other tensiometers were necessary to obtain data relative to the potential gradient to solve the equation of Richards (1931).

The tensiometers (Figure 2) were made of rigid PVC pipe, with porous ceramic cups and nylon tubing (0.002-m internal diameter), used to build the mercury manometer. Mercury manometers were used because of their higher sensitivity to the variations in soil water content.

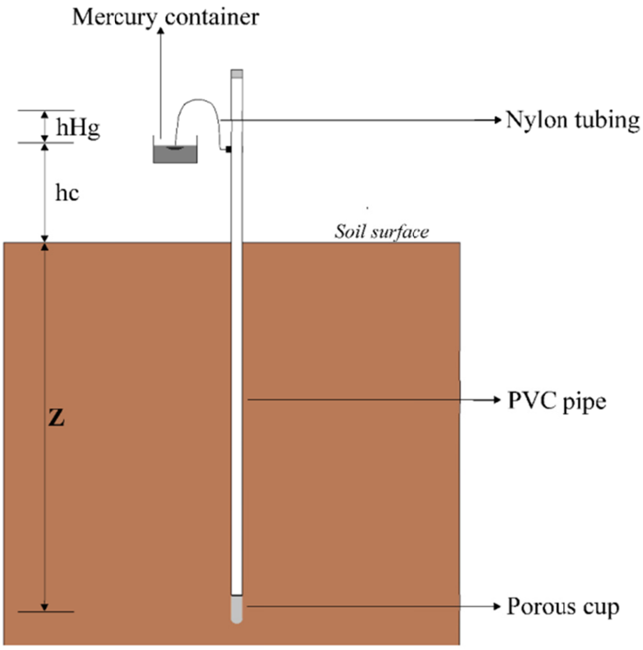

Figure 2. Representation of the scheme of installation and use of the tensiometer. Legend: see Equation (1)

After installing the tensiometers, the plot was wetted to guarantee soil saturation and then covered with a plastic canvas to avoid any water flow through the surface, either evaporation or infiltration. Time zero (t = 0) of water redistribution in the profile was considered as the instant at which the water depth drained from soil surface. After reading the tensiometers at t = 0, during the first 24 hours, the readings were taken every two hours. From this point on, the readings were taken every 24 hours, until drainage virtually ceased.

Tensiometer readings were converted to matric potential (ϕ_m, m), in order to monitor its variation over time, using Equation (1)

$$\phi_m = -12.6h_{Hg} + h_c + z \tag{1}$$

where, h_{Hg} is Hg column height (m), h_c is Hg level height in the container in relation to soil surface (m), z is the installation depth of the tensiometer's porous cup center (m).

Disturbed soil samples were also collected to characterize the soil regarding its granulometric composition (Table 1), with clay content determined through the pipette method (Gee & Bauder, 1986), and its particle density (Blake & Hartge, 1986a). Additionally, undisturbed samples were collected to determine the soil water retention curve (SWRC) (Klute, 1986) and soil bulk density (Blake & Hartge, 1986b).

Table 1. Sand, silt and clay fractions, textural class and soil bulk density in the profile layers

Layers (m)	Sand	Silt	Clay	Textural class	Soil bulk density
	-------------------- g kg^{-1} ---------------------				--------- kg m³ --------
0.0-0.28	873	40	87	Sand	1730
0.28-0.43	843	75	82	Loamy sand	1703
0.43-0.60	585	75	340	Sandy clay loam	1581

Source: Adapted from Freire (2016).

SWRCs were determined in a total of four replicates. In the procedure, saturation water content was considered as equal to soil porosity, obtained by Equation (2),

$$\alpha = 1 - \frac{\rho_s}{\rho_p} \tag{2}$$

where, α is soil porosity (m^3 m^{-3}) and ρ_s and ρ_p are soil bulk and particle densities (kg m^{-3}), respectively.

At low-tension points of the SWRC (0.2; 0.4; 0.6; 0.8 and 1 m), Haines' funnel was used to establish the equilibrium between applied tension and soil water content; for the other points (3.3; 10; 70 and 150 m), the equilibrium was obtained in Richards' porous plate apparatus. Data were fitted to the mathematical model proposed by van Genuchten (1980), Equation (3),

$$\theta = \theta_r + \frac{\theta_s - \theta_r}{[1 + (\alpha|\phi_m|^n)]^m} \tag{3}$$

where, θ corresponds to soil water content ($m^3\ m^{-3}$), θ_r and θ_s are, respectively, residual and saturation water contents ($m^3\ m^{-3}$), ϕ_m is soil water matric potential (m), α is a scaling factor of ϕ_m ($-1/\phi_m$), m and n are fit parameters of the model related to the shape of the curve. The data were fitted using the software Table Curve 2D, trial version 5.01 (SYSTAT, 2014). Empirical parameters were fitted using the Newton-Raphson iterative method, with dependence between m and n.

Soil moisture curve in the field was obtained based on matric potentials measured with tensiometers in the field and on soil-water characteristic curve determined in the laboratory (ϕ_m field-laboratory curve).

2.2 Inverse Modeling with Hydrus-1D

In the version 4.17 of Hydrus 1-D (Šimůnek et al., 2013), the soil profile was divided into three layers (0.0-0.28 m; 0.28-0.43 m and 0.43-0.60 m) with 25 nodes and three points of observation corresponding to the tensiometer installation depths (0.20 m; 0.35 m and 0.50 m) (Figure 3). Iterations were performed by entering the data of matric potential variation over time, from 0 to 330 h.

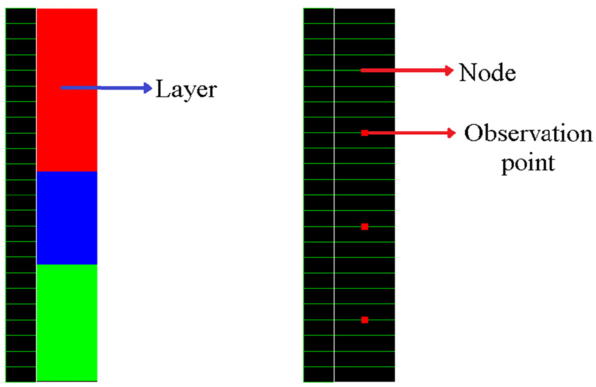

Figure 3. Soil profile division into layers and nodes, and allocation of observation points considered in the inverse modeling procedure

In addition, the software requires the initial, maximum and minimum values of soil hydraulic parameters for each, which are the references on which the entire inverse modeling is based. Boundary conditions were considered as zero flow on soil surface and free drainage at 0.60 m depth. Initial matric potential of the estimate, for each depth and replicate, was set with values as close as possible to zero representing saturated soil.

At 0.35 m depth, target of the present study, the parameters θ_r, θ_s, α and n of the model of van Genuchten (1980) were optimized and, subsequently, the parameter m was obtained based on n ($m = 1 - 1/n$).

2.3 Data Analysis

The parameters of the van Genuchten (1980) model for the 0.35 m depth were compared considering the SWRCs obtained in the laboratory, in four replicates, against the six curves obtained through inverse modeling based on matric potential data over time. Data normality was verified by the Jarque-Bera test and means were compared by Student's t-test for two independent samples, both at 0.05 significance level. Graphs were also constructed with the average curves of laboratory and the one simulated by Hydrus-1D.

In addition, fitted curves of matric potential versus time and soil moisture versus times were also constructed to compare field curves with those simulated by Hydrus-1D. Hydrus-1D performance was evaluated based on the efficiency coefficient € (Nash & Sutcliffe, 1970), Equation (4) and root-mean-square error (RMSE), Equation (5),

$$E = 1 - \frac{\sum_{i=1}^{n}(O_i - P_i)^2}{\sum_{i=1}^{n}(O_i - \bar{O})^2} \tag{4}$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(O_i - P_i)^2}{n-1}} \tag{5}$$

where, O_i corresponds to matric potential data obtained in the field through the instantaneous profile method and P_i to matric potential data obtained through modeling; n is the number of observations and $\bar{O}$ the mean of the values obtained in the field. The same procedure was adopted to compare soil moisture curves over time through ϕ_m field-laboratory curve and through inverse modeling.

For Machado et al. (2003), the Nash-Sutcliffe efficiency coefficient (E) is one of the most efficient to evaluate the fit of hydrological models. This index may vary from negative infinite to 1, and the unit value indicates greater similarity between data sets (ASCE, 1993). RMSE, on the other hand, is used to express the accuracy of the numerical results, exhibiting the value of error in the same unit as the analyzed variable.

3. Results and Discussion

Matric potential variation over time obtained in the field and simulated through inverse modeling is presented in Figure 4. Inverse modeling showed satisfactory performance in the prediction of soil water matric potential over time, given the low RMSE and E value close to one, evidencing good agreement between measured and simulated data.

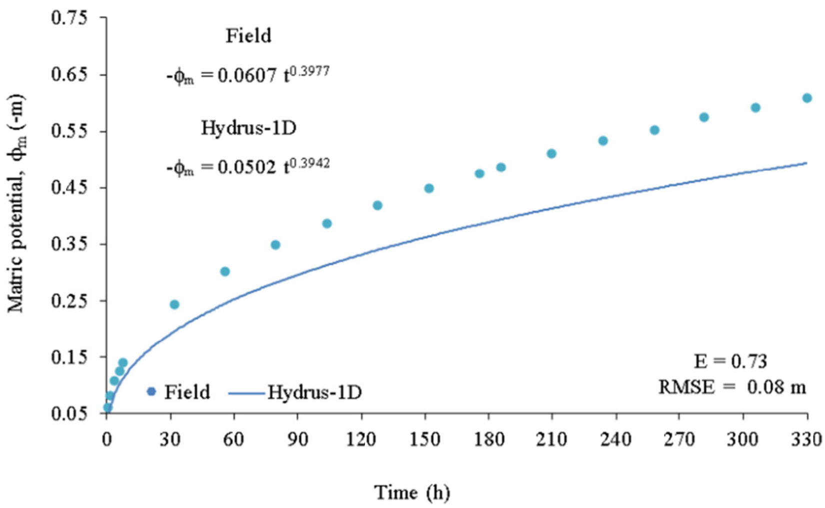

Figure 4. Matric potential over time in the field and through inverse modeling with Hydrus-1D

Root-mean-square error (RMSE) close to zero indicates small error between data simulated by Hydrus-1D and data observed in the field (Peters et al., 2014). In this experiment, Hydrus-1D overestimated matric potential over time and was progressively better towards soil saturation. Despite the increase in the error as water redistribution occurred in the soil up to field capacity, the mean error in this observation range was low, indicating the robustness of inverse modeling in the prediction of soil water energy in the wettest range. Regarding the Nash-Sutcliffe efficiency coefficient (E), one of the important statistical criteria to evaluate the prediction power of hydrological models (Machado et al., 2003), the obtained value, 0.73, demonstrates good similarity between field-measured data and data fitted by inverse modeling.

Figure 5 shows soil moisture over time, obtained in the field and simulated by inverse modeling. As the simulation of matric potential evolution over time, the solution through inverse modeling showed good performance, since the Nash-Sutcliffe efficiency coefficient (E) was equal to 0.77. On the other hand, RMSE was very low, 0.01 $m^3\ m^{-3}$, indicating that Hydrus-1D was efficient in the estimation of soil moisture over time.

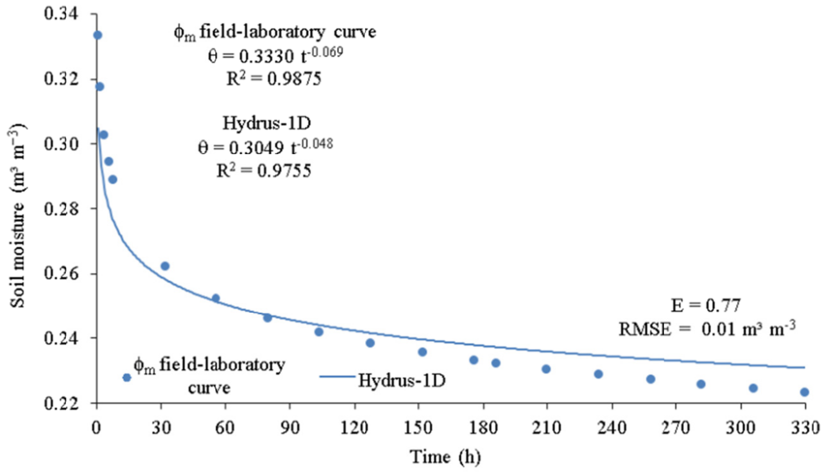

Figure 5. Soil moisture over time through ϕ_m field-laboratory curve and inverse modeling with Hydrus-1D

Although the differences were small, soil moisture was estimated with lower value in the first 70 hours of water redistribution in the soil and higher value from this point on to the end of the experiment, when the inverse modeling protocol was used. As will be discussed hereinafter, given the boundary conditions, soil sample saturation is usually achieved in the laboratory—which will hardly be observed in the field. This explains the greater difference between both protocols in the estimation of total soil porosity when field matric potential is combined with the soil-water characteristic curve obtained in the laboratory.

Although the soil-water characteristic curve determined in the laboratory was significantly different from that obtained using Hydrus-1D based on field data, as will be demonstrated hereinafter, a compensation occurred due to the difference of matric potentials by both procedures (Figure 4), so that soil moisture curves over time became very similar in both methods. However, inverse modeling becomes much more advantageous because it eliminates the procedure of soil samplings and SWRC determination based on them in the laboratory, which demands much more time in comparison to the instantaneous profile-type experiment in the field.

Table 2 shows the means of van Genuchten (1980) equation parameters compared by Student's t-test at 0.05 significance level, considering soil-water characteristic curves obtained in the laboratory and through inverse modeling in the field with Hydrus-1D. The five model parameters significantly differed between both SWRC determination methods.

Table 2. Means of van Genuchten equation parameters, obtained in the laboratory and through inverse modeling with Hydrus-1D in the field, compared by Student's t-test at 0.05 significance level

θ_s (m^3 m^{-3})		θ_r (m^3 m^{-3})		α (m^{-1})		n		m	
Lab	Hydrus	Lab	Hydrus	Lab	Hydrus	Lab	Hydrus	Lab	Hydrus
0.357	0.305	0.079	0.150	11.398	5.062	1.338	1.827	0.252	0.435
14.008*		9.913*		7.164*		2.627*		3.240*	

Note. Lab: Laboratory; Hydrus: Hydrus-1D; * significant difference by Student's t-test at 0.05 significance level; tabulated t at 0.05 significance level = 2.306.

It is important to point out that two curves may be statistically equal even if their parameters are different. On the mathematical aspect, Jorge et al. (2010) report that two soil-water characteristic curves may be considered as equal when their parameters are not different, which was not observed in the studied case. Therefore, it can be claimed that the curves obtained in the laboratory differ from those obtained through inverse modeling with Hydrus-1D. Such claim is important from the practical point of view, because both curves, for being important tools in irrigation management, guide the decision-making differently with respect to soil water management.

Regarding the parameter θ_s, which in the laboratory corresponded to total soil porosity, the mean value found is higher than that obtained through inverse solution. This occurs because undisturbed samples, used in the analytical procedure in the laboratory, in general, are saturated—a situation hardly achieved in the field, which explains the lower value obtained through inverse modeling.

Such assertion is corroborated by Ghiberto (1999), who found saturation moisture contents in the field ranging from 70 to 90% of the total porosity calculated. Therefore, this parameter optimized using field data was expected to show lower value—but the most faithful to the actual situation of maximum moisture obtained in the field. Hence, according to the inverse modeling with Hydrus-1D, only 85% of soil pores were saturated, which corresponds to moisture content of 0.305 $m^3\ m^{-3}$.

Still regarding the difference in the values of saturation, Basile et al. (2003) report that in the laboratory soil hydraulic attributes are obtained in soil samples by imposing a stationary state or transitory conditions that essentially differ from the boundary conditions of field experiments. Although the measurements in the laboratory are more direct and usually easier than those in the field, their validity must be related to the size of the soil sample, which has to adequately represent the heterogeneity of the studied medium. In this case, selecting the appropriate sample size must assume, in the perspective of a comparison between field and laboratory methods, the practicality without losing focus on sample representativeness with respect to the situation in the field.

The mean value of the parameter θ_r obtained with Hydrus-1D was overestimated in comparison to the one obtained in the laboratory. It should be highlighted that the model was provided with data obtained during a 330 h drainage period, until the soil achieved the field capacity condition (insignificant $\partial\theta/\partial t$, ≤ 0,001 $m^3\ m^{-3}\ d^{-1}$). Hence, it is supposed that, since data from wet soil was provided, the model had difficulty estimating the hydraulic behavior of the dry soil, which is evidenced by the high content of residual moisture. Therefore, future studies, including with other instruments, should use data collected in a wider range of time, in order to observe how the Hydrus-1D model behaves with respect to the parameter θ_r.

The empirical parameter α, which represents the inverse of the matric potential at which the largest soil pore cavitates, showed lower mean value when obtained with Hydrus-1D compared with the laboratory procedure. Hence, it can be inferred the model predicts that, in the soil, such phenomenon occurs at lower matric potential than that showed by the laboratory α. The parameters n and m, related to the shape of the curve—for being associated with pore-size distribution—also differ between both methods, evidencing the divergence between soil-water characteristic curves obtained in the laboratory and through inverse modeling with Hydrus-1D.

Figure 6 shows soil-water characteristic curves obtained in the laboratory and through inverse modeling with Hydrus-1D. As previously explained, lower moisture content at saturation was observed in the average curve obtained through inverse modeling, reinforcing the claim that pore saturation is not achieved under field conditions. Therefore, it is reasonable that the curve simulated by Hydrus-1D, particularly from saturation to field capacity, is the one that actually represents the soil in the field, and not the curve determined in the laboratory with boundary condition completely different from the field situation.

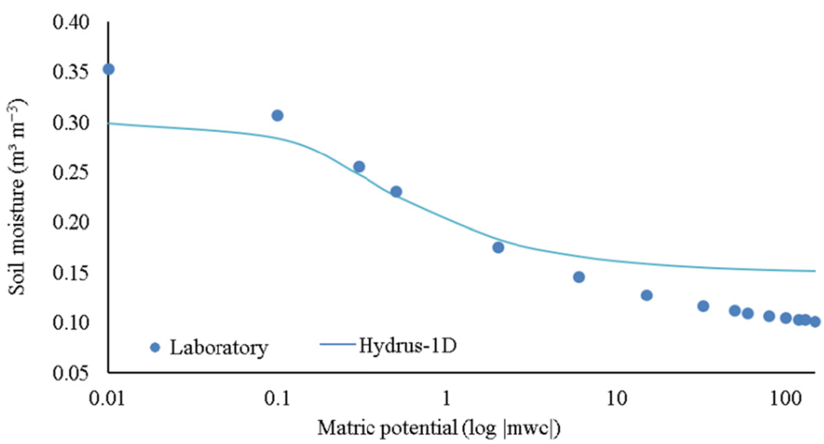

Figure 6. Soil water retention curves obtained in the laboratory and through inverse modeling with Hydrus-1D in the field

In experiment to verify differences in hydraulic attributes in SWCC and in laboratory, Basile et al. (2003) found that, for all studied cases, there was discrepancy between water contents at $\phi_m = 0$ obtained in the field and laboratory, and water retention values were always higher for laboratory curves in the interval between $\phi_m = 0$ and $\phi_m = 1$ m. For these authors, higher water contents at $\phi_m = 0$ for soil samples in cylinders must be attributed to the easy air displacement through the sample under laboratory condition.

According to Figure 6, the differences between the curves are not limited to the wettest portion; the driest portion is also visibly different, especially due to the trend of the inverse model, as previously stated, to overestimate moisture contents in comparison to the laboratory procedure. In this case, for the textural class loamy sand, in which residual moisture content must be low, Hydrus-1D was clearly not efficient to simulate soil moisture at lower matric potentials, probably because the input data were limited to the wet part of the soil.

Considering the results observed in the present study, it is worth pointing out the perception of researchers on field and laboratory methods to estimate soil hydraulic attributes. It is true that many papers in the past were dedicated to the discussion on the validity of soil hydraulic properties obtained in the laboratory for the inference on the hydrological behavior in the field and, as a result, less expensive and less time-consuming techniques have been researched (Basile et al., 2003). However, it is important to highlight that these protocols are not always guaranteed to reliably reproduce what occurs in the field, which explains the stimulus to other approaches—for instance, inverse modeling—in the attempt at better perception on the actual soil hydraulic attributes.

4. Conclusions

In general, the Hydrus-1D model estimates van Genuchten equation parameters and, consequently, the soil-water characteristic curve of an Argissolo more consistently with the field conditions than those obtained in the laboratory.

Hydrus-1D simulates well the behavior of matric potential and soil moisture over time, reducing the time and labor of the procedure to obtain van Genuchten equation parameters in the laboratory.

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