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PEDOFUNCTIONS APPLIED TO THE LEAST LIMITING WATER RANGE TO ESTIMATE SOIL WATER CONTENT AT SPECIFIC POTENTIALS

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KEYWORDS

Soil physics, soil physical quality indicator, available water, pedotransfer functions, artificial neural networks.

ABSTRACT

The least limiting water range (LLWR) is a soil physical quality indicator that receives much attention. It has been criticized and put to the test regarding mathematical models that compose it since they describe the behavior of soil physical attributes in a simplified way. This study aimed to assess the efficiency of some pedofunctions proposed in the literature and artificial neural networks on the accuracy in predicting soil water retention at potentials equivalent to field capacity (θFC) and permanent wilting point (θPWP). In other words, to apply the best models to LLWR of two soil types (Oxisol and Ultisol) and verify changes in their structure. The results indicated that pedofunctions using sand, silt, clay, bulk density, and soil organic matter contents are more efficient in estimating θFC and θPWP. However, the use of multiple linear regression models to predict θFC values below 0.20 $m^3 m^{-3}$ may present a slight tendency to overestimate it, which is not observed in the neural networks. As in R^2, equations from neural networks were more efficient in estimating θFC and θPWP. Pedofunctions used to calculate LLWR differ in the establishment of the critical soil bulk density, exposing the limitations of the model.

INTRODUCTION

Soil physical quality cannot be measured directly, but it is assessed through attributes such as porosity, bulk density, penetration resistance, and water content available to plants (Guimarães et al., 2013). Soil physical quality was better investigated by Letey (1985), who proposed the concept of 'non-limiting water range', which integrates the relationships between soil attributes and water content available to plants. Silva et al. (1994) improved this concept when assembling mathematical models for estimating soil moisture in the field capacity, permanent wilting point, air-filled porosity, and soil penetration resistance, originating a soil structural quality indicator known as least limiting water range. Tormena et al. (1998) later introduced this indicator in Brazil as *Intervalo Hídrico Ótimo*.

The least limiting water range (LLWR) has been received much attention in Brazil and applied in several studies. Among them, Freddi et al. (2009) assessed compaction levels of an Oxisol and its physical quality reduction processes, as well as yield reduction of two maize hybrids as a response to compaction. The authors verified that, at certain levels of soil bulk density, water content should be above the field capacity to avoid limitations due to soil penetration resistance and meet the water requirements of hybrids. In this case, the intense machinery traffic led to soil structural degradation. In addition, the authors proposed soil decompaction actions when bulk density reached 1.46 Mg m^{-3}, considered as critical in LLWR. Betioli Junior et al. (2012) analyzed an Oxisol after 30 years of no-tillage and observed a decrease in LLWR due to an increase in bulk density, regardless of the used critical soil penetration resistance, which was 2 MPa.

Despite the studies that consolidate LLWR as a soil physical quality indicator, it has been criticized and its validity put to the test by several authors (Gubiani et al., 2013, Jong Van Lier & Gubiani, 2015; Cecagno et al., 2016). These studies have questioned the efficiency of the linear mathematical model used to determine LLWR since the relationships between soil attributes are not linear and describe them in a relatively simple way is still one of the challenges of soil physics (Klein et al., 2016; Jong Van Lier & Gubiani, 2015).

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Over the years, researchers have been proposing mathematical models to estimate soil water retention using attributes that correlate directly with one another, such as clay, silt, sand, soil organic matter content, and bulk density (Barros et al., 2013; Medrado & Lima, 2014; Medeiros et al., 2014). These models are also known as pedofunctions or pedotransfer functions (PTF) and can be applied to LLWR.

Most models currently available were developed for temperate regions (Gupta & Larson, 1979; Rawls et al., 1982; Saxton et al., 1986), where edaphoclimatic properties and soil mineralogical characteristics are different from tropical regions. For Brazil, some models have already been established (Reichert et al., 2009, Barros et al., 2013, Medeiros et al., 2014), but their validity in soils submitted to agricultural management different from those of the original database may make them unsuitable for use.

In the case of complex systems, mathematical modeling techniques may be more efficient in predicting soil water content, such as artificial neural networks (ANN) (Jana et al., 2012; Jana & Mohanty, 2012; Nguyen et al., 2017). ANNs have shown high performance due to factors such as robust and parallel distributed structure (layers of neurons), generalization and learning efficiency that make them capable of solving complex problems (Leal et al., 2015). In addition, they are tolerant to outliers, in which they are normalized in the layers of neurons, allowing the modeling of distinct variables and their non-linear relationships. This computational technique simulates the neural structure of intelligent organisms, which acquire knowledge through the experience and acquisition of punctual information.

As an example of the application of ANNs in agricultural research, Leal et al. (2015) reported their efficiency to estimate maize grain yield through soil attributes such as particle size distribution, soil organic matter content, cation exchange capacity, and base saturation. Ebrahimi et al. (2019) compared the efficiency of mathematical models in the estimates of the biological parameters of soil microbiota from their attributes and verified that ANN was more efficient than multiple linear regressions.

Based on these observations, this study aimed to assess the efficiency of some PTFs proposed in the literature and ANNs on the accuracy in predicting soil water retention at potentials equivalent to field capacity (θFC) and permanent wilting point (θPWP). In other words, to apply the best models to LLWR of two soil types (Oxisol and Ultisol) and verify changes in their structure.

MATERIAL AND METHODS

The data were obtained from two representative soils of the Mato Grosso State, Brazil, classified according to the Brazilian Soil Classification System (Embrapa, 2013) as a Dystrophic Red-Yellow Latosol and Dystrophic Red-Yellow Argisol, located at the geographical coordinates 59°11′59.0″ W and 12°35′49″ S and 56°01′16.8″ W and 9°54′04″ S, with an altitude of 350 and 283 m, respectively. According to the U.S. Department of Agriculture (Soil Survey Staff, 2014), the soils are classified as Oxisol and Ultisol, respectively. We will use in this study the USDA classification for standardization purposes.

These soils were sampled from October 2015 to August 2016. The Oxisol was under integrated crop-livestock systems, with an intense crop rotation consisting of soybean as main crop and maize as the second crop intercropped with forage species of the genus *Urochloa*. In some situations, millet or sorghum was chosen instead of maize as the second crop. The forage crops subsidized livestock farming during the dry season until the beginning of rains. The mean annual stocking rate was 2 animals of 450 kg ha^{-1} year^{-1}.

The Ultisol was under *Brachiaria brizantha* cv. Marandu for more than ten years managed for extensive livestock farming, which was not subjected to any soil tillage. The mean annual stocking rate was 1.5 animals of 450 kg ha^{-1} year^{-1}.

Soil physical and chemical attributes were determined from 156 undisturbed and 30 disturbed soil samples. Disturbed soil samples were collected at depths of 0–0.10 and 0.10–0.20 m with a Dutch auger. Undisturbed soil samples were taken using stainless steel volumetric rings with 5 cm high × 5 cm in diameter (98.17 cm^3) from trenches at depths of 0–0.10 and 0.10–0.20 m.

Disturbed soil samples were taken to the laboratory, air dried, and sieved in 200 mm diameter stainless steel mesh sieves. Thus, particle size distribution was determined by the pipette method and organic matter contents (OM) by potassium dichromate oxidation (Embrapa, 2011). Undisturbed soil samples were saturated with water in plastic trays and subjected to tensions of 0, 30, 60, and 100 hPa in a sandbox and 300, 600, 1000, 5000, and 15000 hPa in pressure chambers with a porous plate. After each potential had reached moisture balance, the samples were weighed in order to find the water content. Subsequently, they were subjected to penetration resistance (PR), determined by a bench electronic penetrometer. The penetrometer had the following characteristics: load cell of 20 kg, penetration pin of 3 mm with 4 mm tip in a cone shape with 30° angle, and tip base area of 7.06 mm^2. The constant penetration rate was 10 mm min^{-1}, with two replications per sample, totaling 180 readings per replication. Therefore, the PR data taken from the first centimeter at the top and bottom of the rings were discarded. Thus, each microprofile consisted of PR readings recorded along a vertical transect of 3 cm, acquired from 1 to 4 cm deep, within a core of 5 cm of soil height, in accordance with the representative elementary volume theory. The PR value of each soil sample was obtained from the overall mean of records.

Subsequently, the undisturbed soil samples were oven-dried at 105 °C for 24 hours. The total porosity (TP), bulk density (BD), and soil water content at each tension were calculated (Embrapa, 2011).

For LLWR construction, the model proposed by Busscher (1990) was used to build the PR curve. The water content in which soil penetration resistance is limiting to root growth was obtained by [eq. (1)]:

$$\theta PR = \left(\frac{PRc}{exp^{\beta 1} \times (BD^{\beta 2})}\right)^{\frac{1}{\beta 3}} \quad (1)$$

Where:

θPR is the volumetric soil water content in which PR reaches the critical value (m^3 m^{-3});

BD is the soil bulk density (Mg m^{-3});

PRc is the critical PR value, and

β1, β2, and β3 are the adjustment parameters of the equation. The PRc value of 2 MPa proposed by Taylor et al. (1966) was used.

The water content in which aeration porosity is 10%, i.e., air-filled capacity (θAFC), was found through [eq. (2)]:

$$\theta AFC = TP - 0.1 \quad (2)$$

Where:

TP is the total porosity (m^3 m^{-3}).

For the other LLWR curves corresponding to θFC and θPWP, the pedofunctions proposed by several authors were used, as shown in Tables 1 and 2, respectively.

The multilayer perceptron ANN was also tested. For this, 75% of the data were used for ANN training and 25% for validation. The supervised learning was used with two sets of values, i.e., input and output values. Training consisted of a parameter optimization problem (synaptic weights) to respond to the inputs as expected until the error between observed and estimated values generated by ANNs reached the desired minimum value, i.e., close to zero (Leal et al., 2015).

The ANNs consisted of entries (inputs) corresponding to the soil attributes sand (SD), silt (SIL), clay (CL), BD, and OM. Outputs (response variables) were the respective soil water contents equivalent to θFC and θPWP. We chose the composition of two hidden layers, one with seven neurons and other with five neurons, respectively. Thus, the ANN architecture could be described as 5-7-5-2 (Figure 1). The activation function used was the hyperbolic tangent, as described in [eq. (3)]:

$$TanH = \frac{\sinh(x)}{\cosh(x)} \quad (3)$$

Where:

TanH is the hyperbolic tangent;

sinh is hyperbolic sine,

cosh is hyperbolic cosine.

TABLE 1. Source of pedotransfer functions used to estimate soil water content in the field capacity (θFC).

Source	Soil	Model[1]	R^2
		Oxisol	
Silva et al. (1994)	CAN	$\theta FC = \exp^{-0.873^*} BD^{0.511^*} 100^{-0.115}$	0.96*
Gupta & Larson (1979)	USA	$\theta FC = 0.001^* SD + 0^{ns} ST + 0^{ns} CL + 0^{ns} OM + 0.179^* BD$	0.99*
Rawls et al. (1982)	USA	$\theta FC = -0.588^* + 0^{ns} SD + 0^{ns} ST + 0.027^* CL + 0^{ns} OM + 0^{ns} BD$	0.74*
Saxton et al. (1986)	USA	$\theta FC = \exp[(-1.335^* - \ln A)/B]$	0.57*
Ritchie et al. (1999)	USA	$GM = 0.169^* (CL/SD)^{0.405^*} \rightarrow \theta FC = GM \times BD$	0.47*
Arruda et al. (1987)	BRA	$\theta FC = 0.040^* + 0^{ns} (CL+ST) + 1.22\times10^{-4^*} (CL+ST)^2$	0.74*
van den Berg et al. (1987)	TRP	$\theta FC = -1.752^* + 0.053^* CL + 0^{ns} ST + 0.132^* OM$	0.74*
Oliveira et al. (2002)	BRA	$\theta FC = 0.015^* ST + 0.003^* CL$	0.99*
		Ultisol	
Silva et al. (1994)	CAN	$\theta FC = \exp^{-0.951^*} BD^{-0.163^*} 100^{-0.124^*}$	0.34*
Gupta & Larson (1979)	USA	$\theta FC = 0^{ns} SD + 0^{ns} ST + 0^{ns} CL + 0.017^* OM + 0.109^* BD$	0.99*
Rawls et al. (1982)	USA	$\theta FC = 0.382 - 0.003^* SD + 0^{ns} ST + 0^{ns} CL + 0^{ns} OM + 0^{ns} BD$	0.72*
Saxton et al. (1986)	USA	$\theta FC = \exp[(-0.665^* - \ln A)/B]$	0.60*
Ritchie et al. (1999)	USA	$GM = 0.255^* (CL/SD)^{0.167^*} \rightarrow \theta FC = GM \times BD$	0.01*
Arruda et al. (1987)	BRA	$\theta FC = 0.107^* + 0.003^* (CL+ST) + 0^{ns} (CL+ST)^2$	0.72*
van den Berg et al. (1987)	TRP	$\theta FC = 0^{ns} + 0^{ns} CL + 0^{ns} ST + 0^{ns} OM$	-
Oliveira et al. (2002)	BRA	$\theta FC = 0.004^* ST + 0.006^* CL$	0.97*

[1] CAN: Canadian soils, BRA: Brazilian soils, USA: American soils, TRP: Tropical soils; CL: clay (dag kg^{-1}), ST: silt (dag kg^{-1}), SD: sand (dag kg^{-1}), BD: bulk density (g cm^{-3}), OM: organic matter (dag kg^{-1}), GM: gravimetric moisture at -100 or -15000 hPa (kg kg^{-1}); $A = \exp[-4.396 - 0.0715\, CL - 4.88\times10^{-4} (SD^2) - 4.28\times10^{-5} (SD^2)\, CL]$; $B = -3.14 - 0.002 (CL^2) - 3.48\times10^{-5} (SD^2)\, CL$.

TABLE 2. Source of pedotransfer functions used to estimate soil water content in the permanent wilting point (θPWP).

Source	Soil	Model[1]	R^2
		Oxisol	
Silva et al. (1994)	CAN	$\theta PWP = \exp^{-0.873^*} BD^{0.511^*} 15000^{-0.115}$	0.96*
Gupta & Larson (1979)	USA	$\theta PWP = 0^{ns} SD - 0.017^* ST + 0.010^* CL + 0^{ns} OM + 0^{ns} BD$	0.99*
Rawls et al. (1982)	USA	$\theta PWP = 1.034^* + 0^{ns} SD - 0.099^* ST + 0^{ns} CL + 0^{ns} OM + 0^{ns} BD$	0.95*
Ritchie et al. (1999)	USA	$\theta PWP = \theta_{pwp}{}^* - 1.35\times10^{-10^*} \exp^{(0.285^* SD)}$	0.90*
Arruda et al. (1987)	BRA	$\theta PWP = -0.382^* + 0.013^* (CL+ST)$	0.94*
van den Berg et al. (1987)	TRP	$\theta PWP = 1.034^* + 0^{ns} CL - 0.099^* ST$	0.95*
Oliveira et al. (2002)	BRA	$\theta PWP = 0^{ns} SD - 0.017^* ST + 0.010^* CL + 0^{ns} BD$	0.99*
		Ultisol	
Silva et al. (1994)	CAN	$\theta PWP = \exp^{-0.951^*} BD^{-0.163^*} 15000^{-0.124^*}$	0.34*
Gupta & Larson (1979)	USA	$\theta PWP = 0^{ns} SD + 0^{ns} ST + 0.003^* CL + 0.019^* OM + 0.020^* BD$	0.99*
Rawls et al. (1982)	USA	$\theta PWP = 0.293^* - 0.002^* SD + 0^{ns} ST + 0^{ns} CL + 0^{ns} OM + 0^{ns} BD$	0.70*
Ritchie et al. (1999)	USA	$\theta PWP = \theta_{pwp}{}^* - 2.51\times10^{-5^*} \exp^{(0.087^* SD)}$	0.78*
Arruda et al. (1987)	BRA	$\theta PWP = 0.088^* + 0.002^* (CL+ST)$	0.70*
van den Berg et al. (1987)	TRP	$\theta PWP = 0.088^* + 0.002^* CL + 0.002^* ST$	0.70*
Oliveira et al. (2002)	BRA	$\theta PWP = 0^{ns} SD + 0.003^* ST + 0.005^* CL + 0^{ns} BD$	0.97*

[1] CAN: Canadian soils, BRA: Brazilian soils, USA: American soils, TRP: Tropical soils; CL: clay (dag kg^{-1}), ST: silt (dag kg^{-1}), SD: sand (dag kg^{-1}), BD: bulk density (g cm^{-3}), OM: organic matter (dag kg^{-1}), GM: gravimetric moisture at -100 or -15000 hPa (kg kg^{-1}), θ_{pwp}*: mean water content at the permanent wilting point (m^3 m^{-3}).

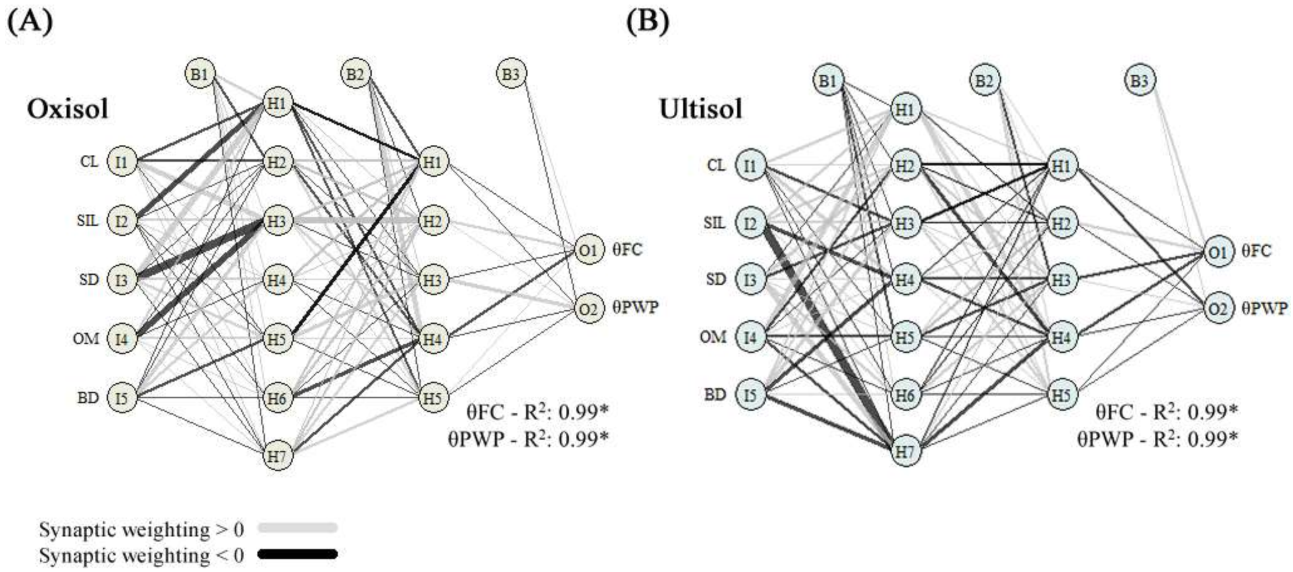

FIGURE 1. Artificial neural network architecture (5-7-5-2) used to estimate θFC and θPWP in an Oxisol (A) and Ultisol (B). Circles with letter B indicate the biases assigned to each layer of neurons, and I, H, and O indicate input attributes, neurons, and outputs of θFC and θPWP, respectively.

The data were submitted to the Shapiro & Wilk normality test (p> 0.05) using the software R (R Development Core Team, 2015). Outliers with values 2.5 times higher than the interquartile range were removed, respecting the limit of 10% of the total observations of each treatment (soil type). Subsequently, a descriptive analysis was performed by calculating the mean, median, minimum, and maximum, standard deviation, coefficient of variation (CV), skewness, and kurtosis. The proposed pedofunctions were adjusted for the respective data sets. The neuralnet package was accessed for ANN training following the previously described criteria for assembly of its structure, using the "plotnet" function for network plotting.

The highest coefficient of determination (R^2) and lowest mean square error (MSE), root mean square error (RMSE), and mean absolute percentage error (MAPE) were used in order to compare the efficiency of pedofunctions in predicting values.

$$MSE=\frac{1}{n}\sum_{i=1}^{n} (e_i-m_i)^2 \quad (4)$$

$$RMSE=\sqrt{\frac{1}{n}\sum_{i=1}^{n}(e_i-m_i)^2} \quad (5)$$

$$MAPE=\frac{\sum_{i=1}^{n}(e_i-m_i)}{\sum_{i=1}^{n}m_i}\times 100 \quad (6)$$

Where:

n is the number of sampling points;

e_i is the value estimated by the pedofunctions, and

m_i is the measured value (observed).

RESULTS AND DISCUSSION

Both soils showed a high BD, with mean values of 1.356 and 1.505 Mg m^{-3} for the Oxisol and Ultisol, respectively (Table 3). Variations of minimum and maximum values of 0.920 and 1.545 Mg m^{-3} for the Oxisol and 1.180 and 1.760 Mg m^{-3} for the Ultisol indicated the existence of potentially compacted sites and sites with a structure not affected by management systems. Based on DB for the construction of pedofunctions, this variability is desirable, as they perform estimates with a wide range of values under previously non-sampled conditions. According to Gomes (2000), the variability of the assessed attributes can be classified according to the magnitude of their coefficient of variation (CV), being considered low when CV is lower than 10%, medium when CV is between 10 and 20%, high when CV is between 20 and 30%, and very high when CV is higher than 30%. Thus, BD variability of the Oxisol was classified as medium, and that of the Ultisol was considered low (14.97 and 8.63%, respectively).

TABLE 3. Descriptive analysis of soil physical and chemical attributes of an Oxisol and Ultisol at a depth of 0.00–0.10 m.[1]

Attributes[2]	Mean	Median	Min	Max	SD	CV	Kurt	Asym	Pw<W
					Oxisol				
SD (dag kg^{-1})	55.341	58.335	52.419	62.424	3.236	5.847	0.057	1.246	0.001*
SIL (dag kg^{-1})	12.527	9.096	8.097	14.266	1.986	15.850	0.185	-1.287	0.001*
CL (dag kg^{-1})	32.131	32.744	29.479	33.315	1.250	3.890	-0.130	-1.181	0.002*
OM (dag kg^{-1})	2.554	2.411	2.333	3.087	0.244	9.553	0.045	1.242	0.001*
BD (Mg m^{-3})	1.356	1.458	0.920	1.545	0.203	14.970	-0.054	-1.209	0.001*
θFC (m^3 m^{-3})	0.285	0.293	0.212	0.346	0.039	13.684	-0.545	-0.558	0.248^{ns}
θPWP (m^3 m^{-3})	0.160	0.168	0.132	0.172	0.014	8.750	-0.170	-1.275	0.000*
					Ultisol				
SD (dag kg^{-1})	65.736	64.900	50.500	81.000	7.019	10.638	0.666	0.502	0.242^{ns}
SIL (dag kg^{-1})	10.932	8.500	1.700	18.900	4.400	36.363	-0.339	-0.268	0.880^{ns}
CL (dag kg^{-1})	22.800	22.300	9.700	39.500	6.560	26.315	0.949	0.296	0.461^{ns}
OM (dag kg^{-1})	3.649	3.562	1.860	7.240	1.546	42.356	-0.289	0.776	0.046*
BD (Mg m^{-3})	1.505	1.361	1.180	1.760	0.138	8.637	0.804	-0.802	0.170^{ns}
θFC (m^3 m^{-3})	0.210	0.209	0.160	0.260	0.043	20.476	-2.214	-0.265	0.002*
θPWP (m^3 m^{-3})	0.160	0.160	0.130	0.220	0.032	20.00	0.563	0.926	0.021*

[1] Min: minimum, Max: Maximum, SD: standard deviation, CV: coefficient of variation (%), Kurt: kurtosis, Asym: asymmetry, Pw<W: p-value of Shapiro-Wilk's test. [2] CL: clay, ST: silt, SD: sand, BD: bulk density, OM: organic matter, Θ_{fc}: soil water content in the field capacity, Θ_{pwp}: soil water content in the permanent wilting point.

The texture of both soils was classified as medium, but the Oxisol presented a higher clay content (Table 1). The range of CL values varied from 29.479 to 33.315 dag kg^{-1} for the Oxisol and 9.700 to 39.500 dag kg^{-1} for the Ultisol, justifying the CV values classified as low and high, respectively. Despite the low variability of clay content in the Oxisol, these values are supposed to be preponderant over the variation of soil water content at specific potentials, especially those related to permanent wilting point.

Regarding OM content, a mean value of 3.649 dag kg^{-1} was observed for the Ultisol and 2.554 dag kg^{-1} for the Oxisol (Table 3). The maximum values indicated the existence of sites with a high decomposition capacity and stability of organic residues (3.087 and 7.240 dag kg^{-1}). The highest OM variability was observed for the Ultisol (42.35%).

Soil water content at equivalent tensions θFC and θPWP presented mean values of 0.285 and 0.160 m^3 m^{-3} for the Oxisol and 0.210 and 0.160 m^3 m^{-3} for the Ultisol, respectively (Table 3). Despite the amplitude of CL contents, θPWP values of both soils were very close. Klein et al. (2013) reported that θPWP is also related to intra-aggregate pores, with BD being the preponderant factor in the amount of cryptopores in soils. The structural units of aggregates are disrupted as BD increases, leading to an increase in textural pores, responsible for water retention at potentials lower than −15000 hPa. In addition, clay increases the specific surface area of the soil matrix, and capillarity and adsorption phenomena determine the matric potential, responsible for soil water retention (Létourneau et al., 2015). Based on these observations, clay content and soil compaction (represented by BD) in these systems may have governed soil water retention conditions, especially in relation to potentials equivalent to θPWP.

The Shapiro & Wilk test confirmed the normal distribution for the attributes CL, SD, and θFC (Table 3). Although it was significant for the other attributes, indicating deviations from normality, the classifications were considered as distribution tending to normality since the mean values were close to the median.

Tables 1 and 2 show the pedofunctions used to estimate soil water contents at specific potentials, theoretically θFC and θPWP. Their respective coefficients of determination showed the quality of model adjustments, with R^2 higher than 0.90 for most cases and all of them significant at 1% probability. A moderate to high correlation was verified between the observed and estimated θFC data (R > 0.74), with a small tendency to overestimate values above 0.30 $m^3 m^{-3}$ and underestimate values below 0.20 $m^3 m^{-3}$ (Figure 2). Although the residuals of pedofunctions generated with soil data from Brazil (Arruda et al., 1987; van den Berg et al., 1987; Oliveira et al., 2002) were higher when compared to the other models, they presented a good performance even without taking into account attributes inherent to edaphology and soil compaction (i.e., OM and BD).

Contrary to what was observed in this study, Bonilla & Cancino (2001) observed a low accuracy for Chilean soils. This limitation was overcome by working on a large database to allow a division of soils into more homogeneous classes. According to Reichert et al. (2009), point scattering is higher and water retention accuracy is lower when using pedofunctions generated from a database with characteristics that differ considerably from soils where the model is assessed. Pedofunctions will only efficiently express water retention of soils with genesis and mineralogy similar to that of the database that was generated (Mecke et al., 2002).

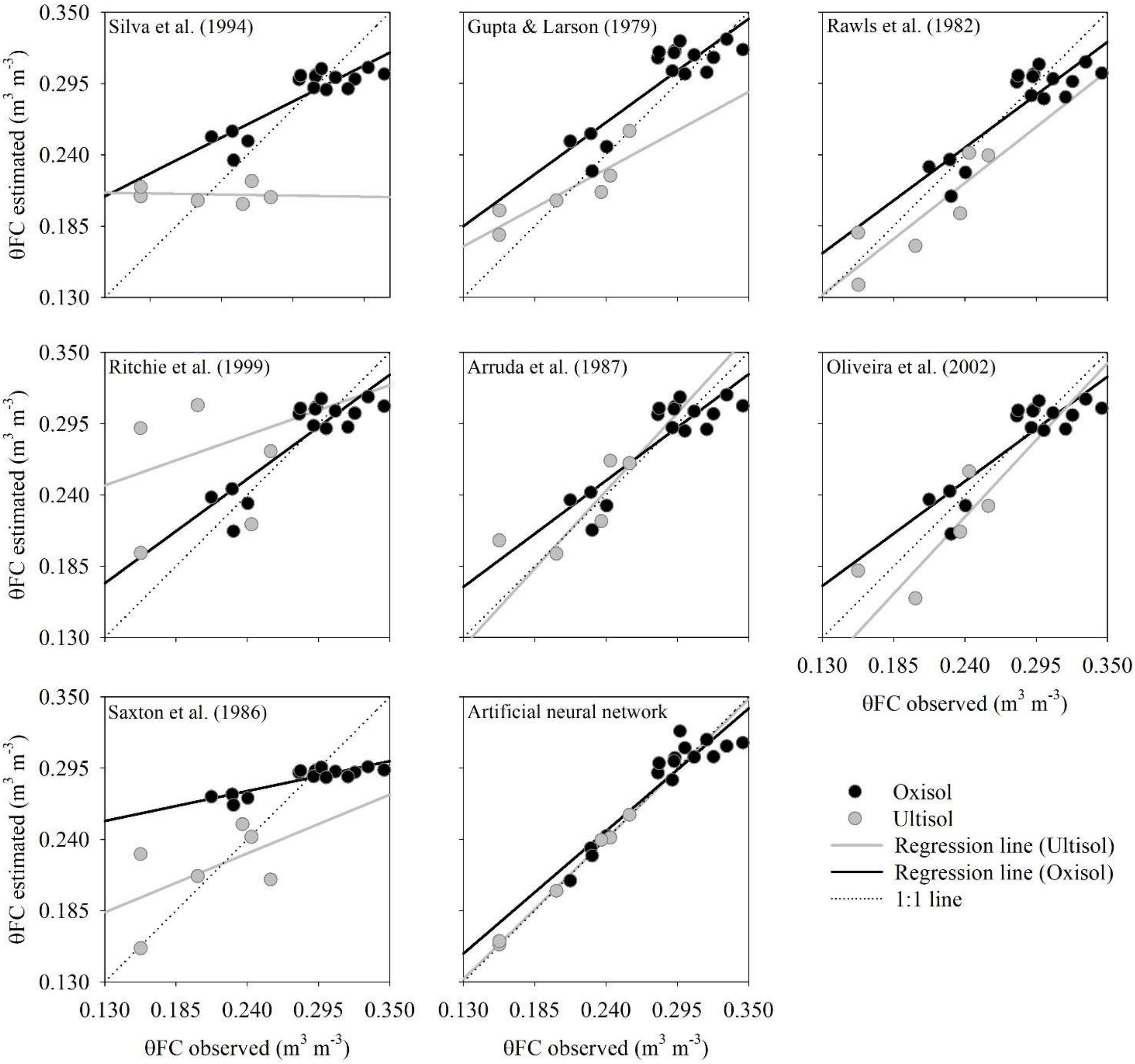

FIGURE 2. Linear regressions between observed and estimated θFC values obtained from the proposed models.

The estimates of θPWP presented lower point scattering and higher accuracy of models when compared to θFC (Figure 3). All tested functions were close to the 1:1 line on a 45° slope, except for the functions of Ritchie et al. (1999) and Silva et al. (1994). This behavior reflected a high correlation of estimates with the observed data due to an R^2 higher than 0.90. In addition, the results showed that changes imposed on the Oxisol by agriculture led to an increase in water volume retained at potentials lower than −15000 hPa, in which θPWP values were higher than 0.16 $m^3 m^{-3}$ in most cases, even in integrated production systems. The estimates of θPWP allowed a more detailed observation of the Oxisol database, in which OM and BD contents were not significant in the pedofunctions of Gupta & Larson (1979), van den Berg et al. (1987), and Oliveira et al. (2002) (Table 2). On the other hand, OM and BD contents were significant in the adjustment of θPWP functions for the Ultisol. According to Rawls et al. (2003), the use of contents of soil organic carbon and their particle size distribution as predictors leads to a small improvement in water content predictions related to the matric potential of −15000 hPa when compared to functions that use only particle size distribution as predictors.

Bonetti et al. (2017) studied the water retention of an Oxisol and Ultisol under integrated crop-livestock systems (ICL) and verified that changes imposed by the management system on soil porosity modified θFC to a higher degree when compared to θPWP. The adequate animal stocking rate and dwell time of the forage crop in ICL can favor the reorganization of porous space by the root system development. This strategy contributes to increasing the water content available to plants, with direct changes in microporosity (Bonetti et al., 2017). In this sense, the management system adopted for the Oxisol (ICL with an intensive crop rotation and high animal stocking rate) may not have been adequate to the maintenance of a pore structure with a diameter lower than 0.2 μm, which favored micropore disruption, directly reinforcing the effect of clay contents under soil compaction conditions. In this case, the function adjustment procedure itself is responsible for maintaining or excluding a certain attribute, aiming at the adequacy of adjustment coefficients, as well as the errors between the generated output patterns to reach the desired minimum value, i.e., close to zero.

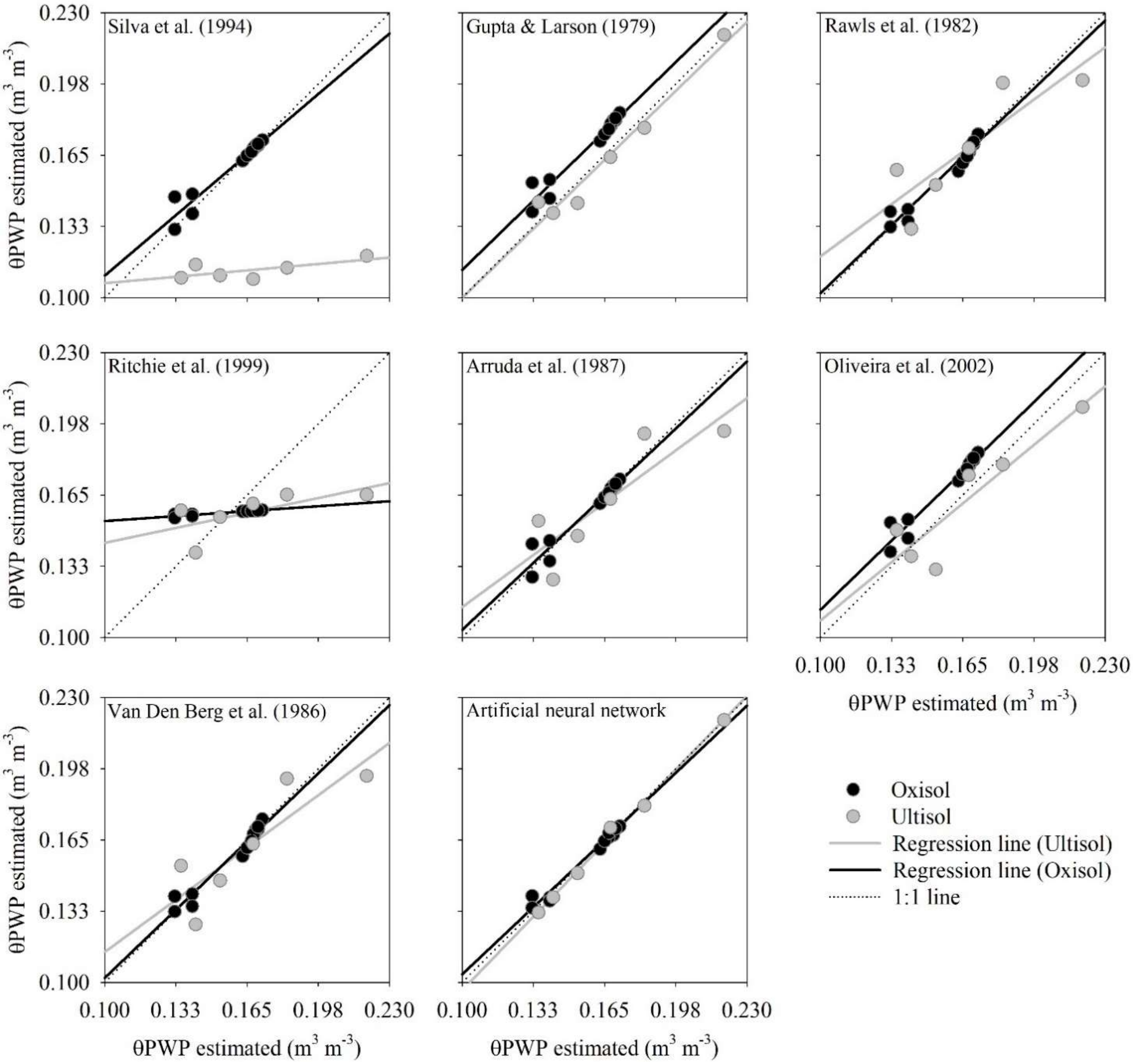

FIGURE 3. Linear regressions between observed and estimated θPWP values obtained from the proposed models.

As in R^2, ANN showed higher efficiency in the estimation of θFC and θPWP. ANN, Arruda et al. (1987), and van den Berg et al. (1987) were the best classified for the MSE, RMSE, and MAPE values of the pedofunctions that estimated θFC (Table 4). On the other hand, ANN, Rawls et al. (1982), and van den Berg et al. (1987), in this order, were the best for those that estimated θPWP. MSE was a sensitive evaluator to errors of pedofunctions because it raised the individual differences between the observed and estimated squared values. This evaluator is always positive and, when zero, indicates the perfect model simulation. In addition to MSE, RMSE also expresses the accuracy of results, with error values under the same dimensions of the analyzed variable. MAPE is a less robust evaluator and showed the error representativeness in relation to the total of the measured observations. In this case, ANNs were classified first in the pedofunctions rank, with lower MSE, RMSE, and MAPE in both θFC and θPWP estimates.

TABLE 4. Mean square error (MSE), root mean square error (RMSE), and mean absolute percentage error (MAPE) calculated from the proposed θFC and θPWP pedofunctions.

Fonte	θFC				θPWP			
	MSE	RMSE	MAPE	Rank[1]	MSE	RMSE	MAPE	Rank[1]
				Oxisol				
Silva et al. (1994)	0.0004	0.0220	0.0118	6th	1.54×10^{-5}	0.0039	0.0075	5th
Gupta & Larson (1979)	0.0005	0.0228	0.0485	7th	0.0001	0.0114	0.0694	6th
Rawls et al. (1982)	0.0004	0.0202	0.0184	5th	9.08×10^{-6}	0.0030	0.0029	2nd
Saxton et al. (1986)	0.0009	0.0304	0.0189	8th	-	-	-	-
Ritchie et al. (1999)	0.0826	0.2875	0.0046	9th	0.0001	0.0135	0.0103	8th
Arruda et al. (1987)	0.0003	0.0192	0.0021	2nd	1.17×10^{-5}	0.0034	0.0004	4th
van den Berg et al. (1987)	0.0003	0.0193	0.0119	3rd	9.08×10^{-6}	0.0030	0.0029	3rd
Oliveira et al. (2002)	0.0003	0.0194	0.0012	4th	0.0001	0.0114	0.0694	7th
Artificial neural network	0.0002	0.0142	0.0018	1st	5.22×10^{-6}	0.0022	0.0019	1st
				Ultisol				
Silva et al. (1994)	0.0016	0.0411	0.0424	7th	0.0036	0.0601	0.3087	8th
Gupta & Larson (1979)	0.0004	0.0222	0.0338	2nd	3.73×10^{-5}	0.0061	0.0121	2nd
Rawls et al. (1982)	0.0006	0.0256	0.0654	4th	0.0002	0.0146	0.0137	3rd
Saxton et al. (1986)	0.0012	0.0359	0.0587	6th	-	-	-	-
Ritchie et al. (1999)	0.0080	0.0895	0.3519	8th	0.0006	0.0254	0.0371	6th
Arruda et al. (1987)	0.0005	0.0229	0.0588	3rd	0.0002	0.0151	0.0170	4th
van den Berg et al. (1987)	-	-	-	-	0.0002	0.0151	0.0170	5th
Oliveira et al. (2002)	0.0012	0.0357	0.0989	5th	0.0008	0.0291	0.0915	7th
Artificial neural network	4.94×10^{-6}	0.0022	0.0043	1st	6.56×10^{-6}	0.0025	0.0096	1st

[1] Rank: classification based in lower MSE, RMSE and MAPE.

The estimates generated by these two adjustment categories could be considered as satisfactory and valid, but the use of multiple linear regression models to predict θFC values below 0.20 m^3 m^{-3} may present a slight tendency to overestimate it, which was not observed by the neural network. The pedofunctions applied to LLWR showed that the available soil water content (AW), represented by the difference between θFC and θPWP, was positively influenced by an increase in BD between 0.69 and 1.06 Mg m^{-3} in all cases (Figure 4C, D). This behavior confirms the positive relationship between soil compaction and the available water range (without considering restrictions imposed by θPR), in which the water content retained at potentials of −100 and −15000 hPa is higher. The models proposed by Silva et al. (1994) and Ritchie et al. (1999) stood out from the other pedofunctions in both soils, indicating an excess LLWR of 0.02 m^3 m^{-3} in the Oxisol (Figure 4A) and a deficit of 0.04 m^3 m^{-3} in the Ultisol (Figure 4B) based on the estimates carried out by ANN, which had the best performance in both soils.

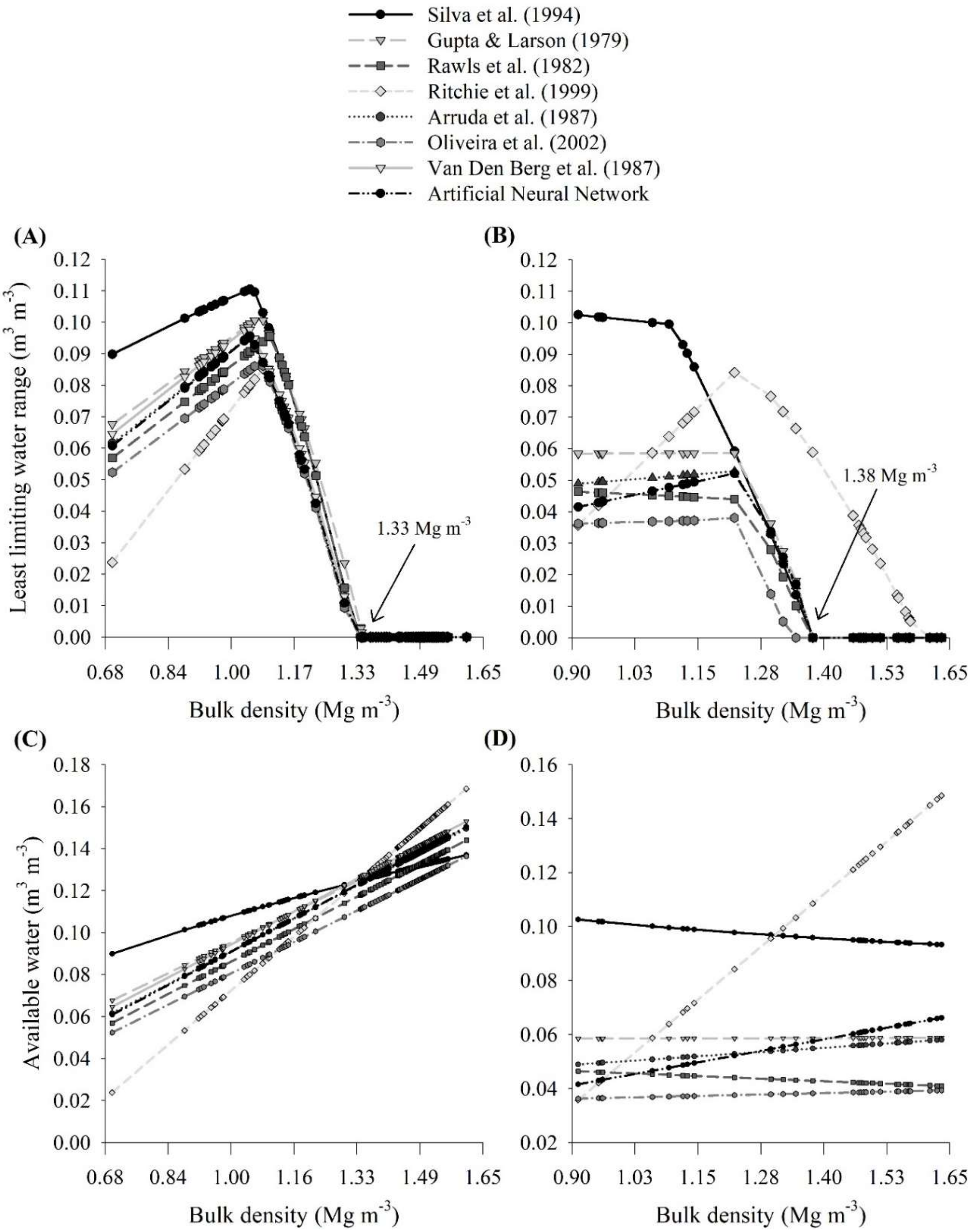

FIGURE 4. Variation of LLWR in the Oxisol (A) and Ultisol (B) and available water content in the Oxisol (C) and Ultisol (D) using the tested pedofunctions.

Regarding the critical BD, in which LLWR is zero, all the proposed models for Oxisol showed LLWR zero for a BD of 1.33 Mg m^{-3}, while most of the models for the Ultisol presented LLWR zero for a BD of 1.38 Mg m^{-3} (Figure 4A, B). In this case, the models of Oliveira et al. (2002) and Ritchie et al. (1999) underestimated and overestimated the critical BD in the Ultisol, respectively. For LLWR construction in the Ultisol using the pedofunctions proposed by Oliveira et al. (2002), the critical BD would be 1.35 Mg m^{-3}, while using the pedofunctions proposed by Ritchie et al. (1999), the critical BD would be 1.61 Mg m^{-3} (Figure 4B). Considering that LLWR accesses soil physical quality through BD, the main objective of its determination is to clarify the critical BD so that preventive actions are taken in agricultural systems. In the evaluated systems, the θPR curve was the preponderant factor in the establishment of the critical BD.

Regardless of the pedofunctions used for LLWR construction in the Oxisol, it was not restricted by the air-filled capacity curve (θAFC) (Figure 5). The θAFC was above θFC in all cases, not being a preponderant factor even at high BD levels. According to Gubiani et al. (2013), there are practically no criticisms reported in the Brazilian literature for the upper LLWR limits. Most crops are grown on soils with optimum drainage, where the period of water excess, i.e., soil aeration deficiency is much lower when compared to periods of water deficit. Under these soil conditions, studies have indicated a higher relationship of plant development with PR (Freddi et al., 2009; Kaiser et al., 2009), being more frequent than with θAFC.

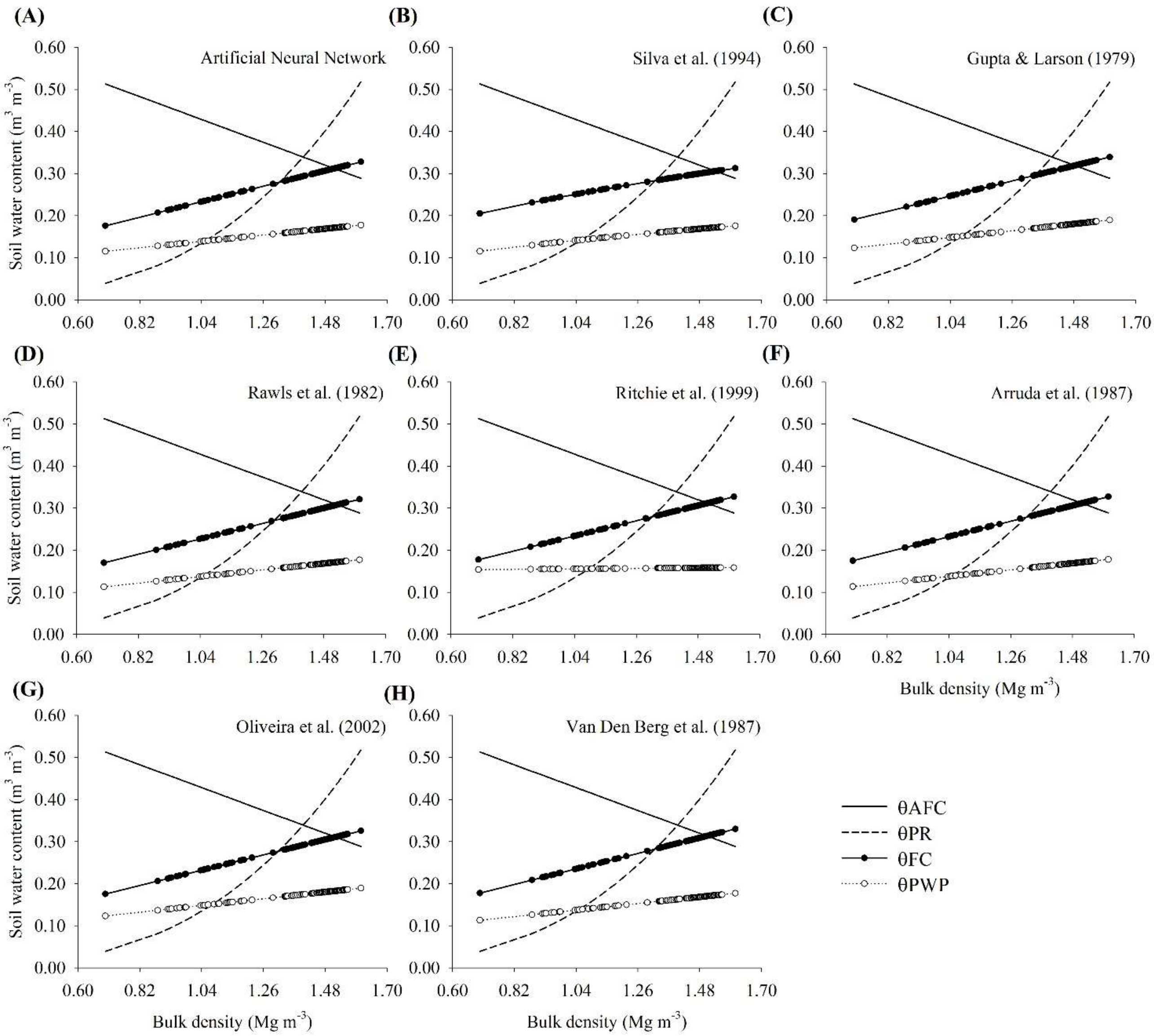

FIGURE 5. LLWR construction of the Oxisol as a function of soil bulk density using the proposed pedofunctions to estimate θFC and θPWP.

When the proposed pedofunctions are used to construct the LLWR concept, it is evident that the main changes occur on the available soil water content (AW). In the Oxisol, LLWRs estimated by ANN, Gupta & Larson (1979), Rawls et al. (1982), Ritchie et al. (1999), Arruda et al. (1987), Oliveira et al. (2002), and van den Berg et al. (1987) were similar (Figure 5). The model presented by Silva et al. (1994) overestimated AW values for conditions of lower bulk density, i.e., between 0.75 and 1.2 Mg m^{-3} (Figure 5B). In contrast, the model of Ritchie et al. (1999) underestimated AW at low BD levels and then presented significant AW gains with an increase in BD (Figure 5E).

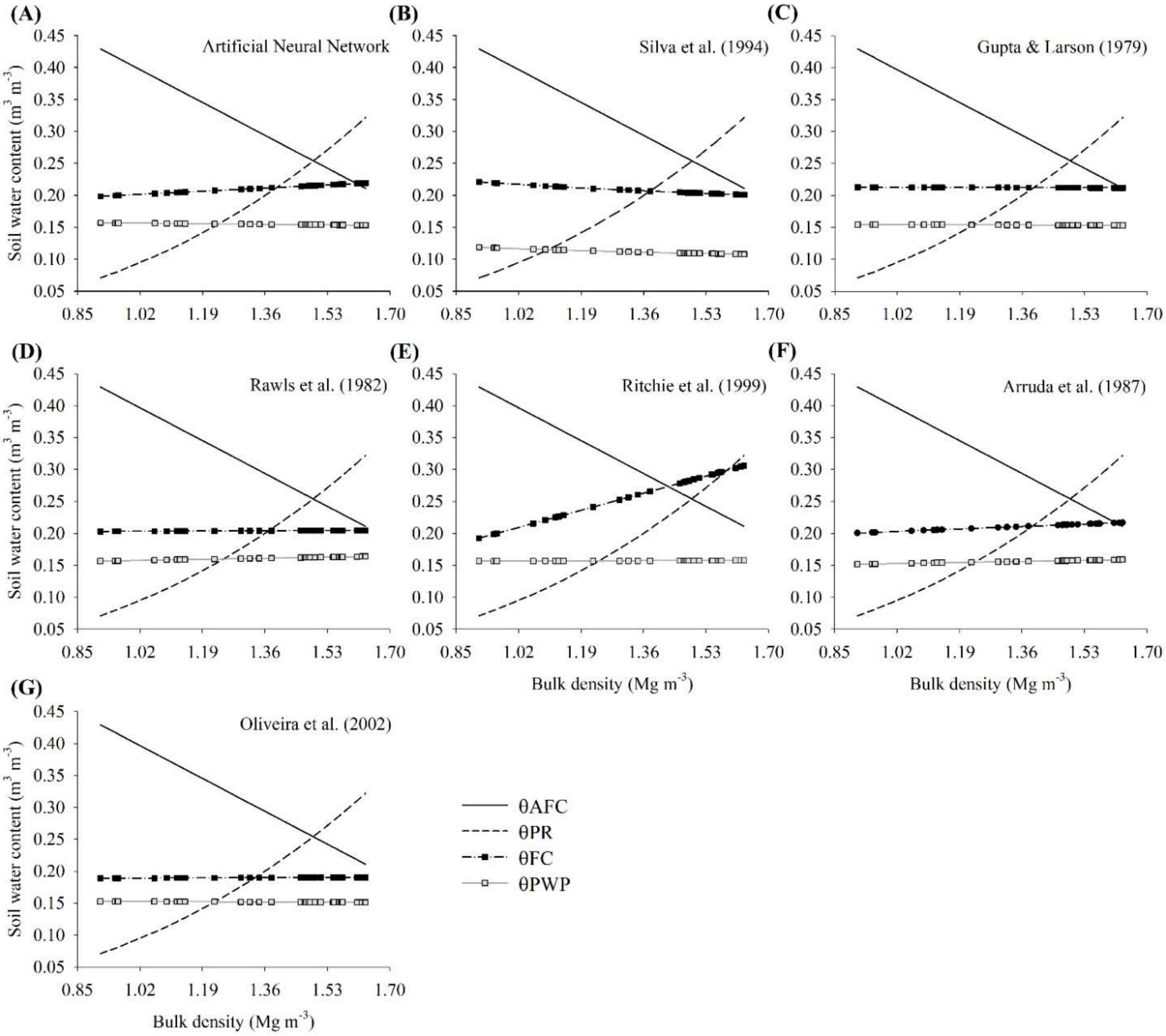

FIGURE 6. LLWR construction of the Ultisol as a function of soil bulk density using the proposed pedofunctions to estimate θFC and θPWP.

Considering the results obtained for the Ultisol, it was evident that AW was overestimated under all BD conditions when the pedofunctions proposed by Silva et al. (1994) were used (Figure 6B). The model proposed by Ritchie et al. (1999), as observed for the Oxisol, underestimated AW at low BD levels and overestimated AW at high BD levels, which would restrict its use for this type of soil (Figure 6E).

The results obtained in this study provided important information for the management of compacted and/or irrigated areas, demonstrating the use of the main models to estimate θFC and θPWP, the result on LLWR determination, and available water of two soils frequently found in Brazil. In addition, further studies using a larger database are needed, allowing the establishment of an artificial neural network that could be validated for Brazilian soils or tropical regions.

CONCLUSIONS

Among the evaluated pedofunctions, multilayer perceptron artificial neural networks are more efficient to estimate water contents in the field capacity and permanent wilting point.

Pedofunctions that use contents of sand, clay, organic matter, and soil bulk density are more efficient in estimating water contents in the field capacity and permanent wilting point.

Multiple linear regression techniques are inferior regarding statistics that measure the accuracy of models and tend to overestimate water content values in the field capacity.

Pedofunctions differ in the establishment of the critical bulk density when they are used to calculate the least limiting water range, exposing the limitations of the models.

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