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Estimation of Saturated Volumetric Moisture of Brazilian Soils for Sustainable Water Management in Agriculture

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ABSTRACT
Pedotransfer functions are used to estimate soil hydraulic characteristics, which are laborious and involve high costs, especially in a country of continental dimensions like Brazil. Since the determination of saturated volumetric humidity helps with the sustainability of the water used in agriculture, avoiding waste, the present work aspired to develop a new pedrotransfer function to predict said property for Brazilian soils using HYBRAS data. A total of 1053 soil samples from the North, Northeast, Midwest, Southeast and South of the country were considered, for which the database informs the hydraulic parameters of each sample collected. Using the Multiple Linear Regression method, the function was developed from the value of the density measured in loco and the fractions of sand and clay, having been validated through the comparison of the results with those obtained by models available in the literature. When compared to existent pedotransfer functions, the new function obtained a sufficient behavior, presenting values close to the ideal ones for the following parameters: Mean Square Error, Model Efficiency, Residual Mass Coefficient and Deviation Ratio. Thus, it can be applied to the different Brazilian soils present in the database used.

KEYWORDS: Water resources management. Pedotransfer function. HYBRAS.

1 INTRODUCTION

In the agriculture sector, the knowledge of the soil hydrodynamic properties is extremely important. Andrade et al. (2020) state that this is a fundamental area of Soil Science, since it has an influence on the dynamics of water throughout the agricultural production process. Considering that this sector, supported by the production under irrigation, is the great consumer of water in the world, since this resource is essential for its development, its administration and proper control will provide plantings and crops in a fair and balanced way (PAZ; TEODORO; MENDONÇA, 2000).

In this sense, the knowledge about the saturated volumetric moisture has its use to choose the cultivations compatible with the target regions, being a parameter used in the irrigation management in order to prevent water waste. A saturated soil, that is, flooded, does not present a favorable condition for the development of many plant species, since all voids are filled with water, which limit the essential supply of oxygen for the development of the roots and with the continuity of irrigation on a land in this condition, all excess water will be lost (LACERDA, 2007; PAZ; TEODORO; MENDONÇA, 2000).

However, according to Veloso (2021), the determination of soil physical and hydric properties may require costly and laborious tests, which boosts the development and use of Pedotransfer Functions (PTF). These are mathematical applications that estimate difficult-to-obtain soil hydrodynamic properties from other more easily and economically measured data, such as percentages of sand, clay, and silt. In the last three decades, PTFs have been used more for soils in temperate climates and less for those in tropical climates. This divergence can be attributed to the lack of large-scale databases. In the case of Brazil, it is due to the fact that it is a country of large territorial size, with a great variability of climate and soil typologies (SOARES; HOLANDA; OLIVEIRA, 2022; COSTA; SOARES, 2019).

In view of this, Ottoni et al. (2018) developed a hydrophysical database from Brazilian soils (Hydrophysical Database for Brazilian Soils - HYBRAS) for the development of pedotransfer functions. Available free of charge, the purpose of the researchers was to provide data for the creation of more suitable functions for regions with tropical conditions, such as those found in Brazil.

2 OBJECTIVES

The purpose of this article was to use the HYBRAS database for the development of an PTF to predict saturated volumetric moisture through multiple linear regressions and compare its performance with other functions available in the literature. With the development of this new function, it is intended to provide a tool to help reduce water waste in agriculture.

3 METHODOLOGY

The proposed PTF was created based on data from 1075 samples available in the HYBRAS database. This database was developed to provide data on the hydraulic characteristics of the soils from 445 locations in the country for simulation models. The database tables present general information of each soil sample, such as location and pathological classification, physical attributes of the samples, saturated hydraulic conductivity, saturation moisture, total porosity, volumetric water content data and results of the parameters of the Van Genuchten function of the soils of 15 Brazilian states: Rio Grande do Sul (316), São Paulo (183), Rio de Janeiro (115), Goiás (98), Santa Catarina (75), Minas Gerais (61), Amazonas (60), Bahia (56), Pará (55), Maranhão (27), Mato Grosso do Sul (12), Pernambuco (5), Sergipe (5), Ceará (5) and Espírito Santo (2) (OTTONI, 2018).

The large number of data available for the South and Southeast regions should be emphasized – totaling 391 and 363 samples, respectively – when compared to the Northeast, Midwest and North regions, which together add 321 samples. This data distribution scenario highlights the need for more research to obtain data for the three regions closest to the Equator.

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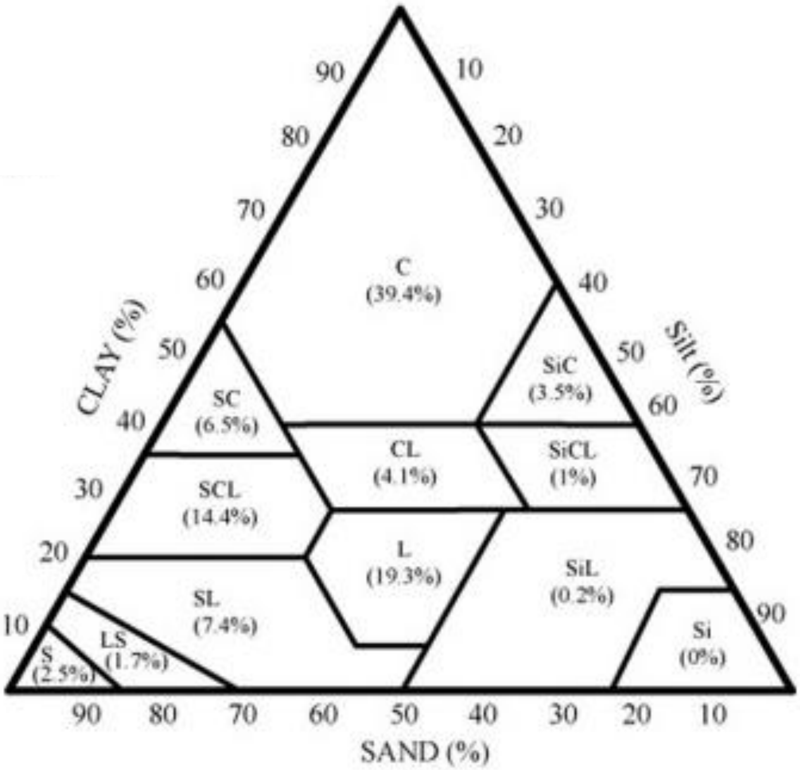
Figure 1 - HYBRAS data textural classification triangle



Source:Ottoni, 2018

3.1 Data definition

To determine the Proposed Model (PM) for the saturated volumetric moisture (θs), the dry soil density (D) and the fractions of clay (Cly), sand (Snd) and silt (Sil) were used as basis, according to the covariance and correlation between them, expressed in Tables 1 and 2. We disregarded other parameters available in HYBRAS, such as organic matter, due to the absence of data for some sites.

Table 1 - Covariance between variables

	Saturated Moisture	Density	Sand	Clay	Silt
Saturated Moisture	0.011				
Density	-0.025	0.074			
Sand	-0.015	0.032	0.045		
Clay	0.014	-0.031	-0.033	0.040	
Silt	0.001	-0.001	-0.012	-0.007	0.019

Source: authors

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Table 2 - Correlation between variables

	Saturated Moisture	Density	Sand	Clay	Silt
Saturated Moisture.	1				
Density	-0.861	1			
Sand	-0.645	0.557	1		
Clay	0.636	-0.572	-0.780	1	
Silt	0.076	-0.033	-0.417	-0.243	1

Source: authors

After the selection of these parameters, tests were performed from the establishment of combinations between each one, applying the Multiple Linear Regression method in order to define the most efficient PTF.

For this, however, of the 1075, 10 samples were discarded because they presented a value equal to zero for one of the stipulated variables (observations 259, 262, 263, 265, 316, 315, 325, 331 and 332) and other 12 were excluded because they did not have data on density (comments 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 317 and 330). Thus, 1053 samples of the total data set were used, of which 842 (80%), randomly defined, were used for the construction of the model and other 211 (equivalent to 20%), for its validation.

The most significant model was established, a priori, due to the p-value of the variables considered, the adjusted coefficient of determination (adjusted R^2) and the standard error of the regression. The p-value needed to be below the significance level α = 0.05, the adjusted R^2 should be as close to 1 (or 100%) and the standard error as close to 0.

3.2 Model Validation

This step consisted of comparing the saturated moisture values obtained for the Proposed Model and for the models produced by Vereecken et al. (1989), Ghorbani and Homaee (2004), Barros et al. (2013), Costa and Soares (2019) and Soares, Holanda and Oliveira (2022), whose equations make use of the same parameters chosen for the MP and are described below.

3.2.1 Vereecken's model et al. (VE)

Developed by Vereecken, Maes, Feyen and Darius, this PTF was stipulated for 40 series of Belgian soils, considering the bulk density of the soils (g/cm3) and the percentage of clay. (VEREECKEN et al., 1989).

$\theta s = 0{,}81 - 0{,}283\ D + 0{,}001\ Cly$ Eq. 1

3.2.2 Ghorbani and Homaee Model (GH)

Ghorbani and Homaee's PTF considers sand percentage and bulk density (g/cm³) and is based on data from 34 randomly defined European soil samples (GHORBANI; HORMAEE, 2004).

$\theta s = 0{,}933 - 0{,}000707\ Snd - 0{,}311\ D$ Eq. 2

3.2.3 Barros et al. (BR)

The pedotransfer function defined by Barros et al. (2013) results from the study of 786 soil samples from the Brazilian Northeast Region, of which 85% were used to estimate the PTF and 15% for its validation, considering the percentages of sand and clay.

$\theta s = 0{,}5526 - 0{,}2320\ Snd - 0{,}1178\ Cly$ Eq. 3

3.2.4 Costa and Soares (CS)

Costa and Soares (2019) produced the following PTF for 83 Brazilian soil samples, admitting the percentages of clay and sand and the density value (g/cm³).

$\theta s = -0{,}00115\ Cly - 0{,}31209\ D^2 + 0{,}990718\ D - 0{,}00158\ DSnd$ Eq. 4

3.2.5 Soares, Holanda and Oliveira (SHO LI / SHO NL)

The model was elaborated from the 1075 samples of the HYBRAS data set and the authors developed a linear function (Eq. 5) and a non-linear function (Eq. 6) to estimate the saturated moisture of Brazilian soils.

SHO LI: $\theta s = 0{,}6857\ Cly + 0{,}2561\ Snd + 0{,}0987\ D$ Eq. 5

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SHO NL: $\theta s = 0{,}8544\ Cly - 0{,}6613\ Cly^2 + 0{,}0034\ Cly^{-1} - 0{,}3815\ ClySnd +$
$+ 0{,}2533\ D - 0{,}0790\ D^2 + 0{,}1669\ D^{-1} - 0{,}3245\ DSnd$ Eq. 6

After calculating the saturated humidity from the Proposed Model and the models used for comparison, some statistical parameters were calculated to attest to the prediction capacity of the PM in relation to the others, namely: absolute error, Mean Squared Error (MSE), Efficiency of the Model (EM), Residual Mass Coefficient (RMC) and Ratio of Deviations (RD) (Eq. 7 to 11). The last five have as reference values, respectively: 0, 0, 1, 0 and 1.

$$| error | = \sqrt{(M_i - T_i)^2} \quad \text{Eq. 7}$$

$$MSE = \frac{\sqrt[100]{\frac{\sum_{i=1}^{N}(T_i - M_i)^2}{N}}}{\bar{M}} \quad \text{Eq. 8}$$

$$EM = \frac{\sum_{i=1}^{N}(M_i - \bar{M})^2 - \sum_{i=1}^{N}(T_i - \bar{M})^2}{\sum_{i=1}^{N}(M_i - \bar{M})^2} \quad \text{Eq. 9}$$

$$RMC = \frac{\sum_{i=1}^{N}(M_i - \sum_{i=1}^{N} T_i)}{\sum_{i=1}^{N} M_i} \quad \text{Eq. 10}$$

$$RD = \frac{\sum_{i=1}^{N}(M_i - \bar{M})^2}{\sum_{i=1}^{N}(T_i - \bar{M})^2} \quad \text{Eq. 11}$$

Where: Ti are the calculated values, Mi the measured, $\overline{\mathrm{M}}$ the average of the measured values, and N the total number of observations.

With the results, each model was classified from 1st to 7th place according to the greater or lesser proximity of the values obtained in relation to the reference values. The final score corresponds to the sum of the positions earned for each parameter.

4 RESULTS AND DISCUSSIONS

4.1 Proposed Model

The tests that were performed to choose the most appropriate function for the prediction of saturated moisture, and for which the validation steps were performed, are summarized in Table 3 below. It contains the adjusted R² and the standard error of each regression, as well as the resulting function and the numbering of the test according to the order in which it was performed.

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Table 3 - Summary of results found for the most significant tests for the Proposed Model

TEST	R^2 adjusted	Standard Error	Function
1	0.7840	0.0497	$\theta s = 0,8914 - 0,2783\ D - 0,0894\ Snd + 0,0480\ Cly$
2	0.7920	0.0488	$\theta s = 0,8049 - 0,2113\ D + 0,1703\ Are + 0,0486\ Arg - - 0,1883\ DAre$
3	0.8010	0.0476	$\theta s = 1,0427 - 0,3807\ D - 0,0993\ Snd - 0,3504\ Cly + + 0,2952\ DCly$
4	0.7850	0.0495	$\theta s = 1,0142 - 0,2407\ D - 0,2681\ Snd - 0,1231\ Cly - 0,1264\ DSil$
5	0.8020	0.0475	$\theta s = 1,1031 - 0,4888\ D - 0,0963\ Snd - 0,3641\ Cly + + 0,3156\ DCly + 0,0419\ D^2$
10	0.7810	0.0499	$\theta s = 0,9357 - 0,4176\ D + 0,1029\ DCly + 0,0402\ D^2$
12	0.7890	0.0491	$\theta s = 0,8970 - 0,2938\ D - 0,0737\ Snd + 0,0564\ DCly$
14	0.7940	0.0485	$\theta s = 1,0027 + 0,2171\ Snd + 0,0655\ Cly - 0,2196\ DSnd - 0,4248\ \sqrt{D}$
15	0.9459	0.1144	$\theta s = 0,0737\ D + 0,2612\ Snd + 0,7220\ Cly$
16	0.9722	0.0811	$\theta s = 0,2641\ D + 1,5686\ Snd + 0,3471\ Cly - 1,0906\ DSnd$
17	0.9662	0.0898	$\theta s = 0,2080\ D + 0,1050\ Snd + 1,6156\ Cly - 0,9291\ DCly$
18	0.7916	0.0488	$\theta s = -1,4247 - 4,2018\ D - 0,3963\ Cly + 0,3883\ DCly + 0,1457 D^{-1} + 5,5641\ \sqrt{D} + 0,5363\ D^2$
19	0.8043	0.0473	$\theta s = 0,4256 - 2,0107\ D - 0,0946\ Snd - 0,4628\ Cly + 0,3867\ DCly + 1,9872\ \sqrt{D} + 0,2735\ D^2$
20	0.9897	0.0473	$\theta s = - 2,93771\ D - 0,09301\ Snd - 0,42419 Arg + 42419\ DCly + 3,21081\ \sqrt{D} + 0,41320\ D^2$

Source: authors

After checking all the equations described above and considering the one with the highest adjusted R^2 and lowest error and p-value lower than 0.05 for all variables, the function resulting from test number 20 was adopted as the Proposed Model, as shown in Eq. 12.

$$\theta s = - 2,93771\ D - 0,09301\ Snd - 0,51488\ Cly + 0,42419\ DCly + 3,21081\ D + 0,41320\ D^2 \qquad \text{Eq. 12}$$

The graph Measured Volumetric Moisture × Calculated Volumetric Moisture (Figure 2) shows that the results obtained by the Proposed Model, represented by the blue triangle,

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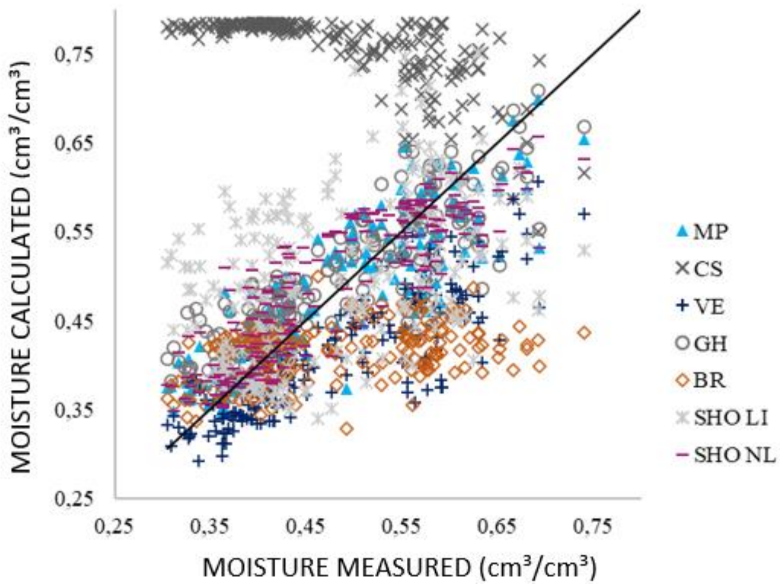
and by the SHO NL Model, represented by the magenta dash, are closer to the trend line, which indicates a better accuracy in determining the saturated volumetric moisture from the data provided, using the equations proposed by the two models. Regarding the linear function of Soares, Holanda and Oliveira (2022), one notices greater dispersion of the data when compared to PM., VE, GH, BR e SHO NL. The most discrepant behavior is attributed to CS Model, whose results remained far from the trend line in comparison to the results of the other six studied models.

Figure 2 - Measured Volumetric Moisture x Volumetric Moisture Calculated by PTFs



Source: authors

Comparing the absolute errors for each model, and considering the error interval ranging between 0.01 and 0.5 - the Table 4, arranged below, shows the percentage of errors lower than those specified for each function used.

Table 4 - Percentage of absolute errors below the established range

Error (e)	PM	VE	GH	BR	CS	SHO LI	SHO NL
e ≤ 0,5	100,00%	100,00%	100,00%	100,00%	100,00%	100,00%	100,00%
e ≤ 0,3	100,00%	100,00%	100,00%	98,58%	47,87%	99,05%	100,00%
e ≤ 0,2	100,00%	96,21%	100,00%	91,47%	29,38%	93,84%	100,00%
e ≤ 0,1	95,73%	74,41%	92,89%	63,03%	7,11%	63,03%	94,79%
e ≤ 0,05	72,51%	45,50%	63,51%	41,71%	2,84%	38,39%	65,40%
e ≤ 0,01	21,80%	6,16%	9,48%	12,32%	0,47%	7,11%	19,91%

Source: authors

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Analyzing Table 4, it is possible to see that both the function obtained for the Proposed Model and both GH and SHO NL models had 100% of errors lower than 0.2. However, for the other values, the PM showed better performance than the others, with the largest error equal to 0.1615 cm^3/cm^3.

For the proposed model, in the 46 observations whose errors were less than 0.01, there was a predominance of albaqualf. One hundred and seven observations had errors between 0.01 and 0.05, of which 29 of them correspond to latosols of clayey texture, sandy clay and sandy loam, 22 correspond to planosols of textures of equivalent fractions and 21 to clayey texture. Among the 49 samples with errors between 0.05 and 0.1, 29 are constituted by latosols of clayey texture, sandy clay and sandy loam. Among the 9 observations whose errors were greater than 0.1, there was a predominance of clayey latosols. The concentration of the smallest errors was in the state of Rio Grande do Sul, whereas the largest errors belonged to samples from the state of São Paulo.

The results for the parameters MSE, EM, RMC, and RD are broken down in Table 5. In two of the four, MSE and RMC, the Proposed Model has responses closer to the benchmarks, again, followed by SHO NL.

Table 5 - Obtained values of MSE, ME, RMC and RD for the analyzed functions

	PM	VE	GH	BR	CS	SHO LI	SHO NL
MSE	1,95	1,97	1,95	1,98	2,02	1,98	1,95
EM	0,97	0,96	0,97	0,98	0,68	0,97	0,97
RMC	0,00	0,14	-0,03	0,14	-0,56	-0,03	-0,02
RD	31,65	25,06	39,56	-0,03	3,16	29,72	34,43

Source: authors

The analysis of the efficiency of the model is finalized with the assembly of the ranking, taking into account the results of Table 5. From the analysis of Table 6, it is possible to verify that the Pedotransfer Function developed in this work obtained less points, which means it has achieved better placement in most parameters and is therefore able to safely estimate saturated moisture for Brazilian soils.

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Table 6 - Classification of models according to EQM, MSE, ME, RMC and RD

	MP	VE	GH	BR	CS	SHO LI	SHO NL
MSE	1º =	4º	1º =	5º =	7º	5º =	1º =
EM	3º =	2º	3º =	7º	1º	3º =	3º =
RMC	1º	5º =	3º =	5º =	7º	3º =	2º
RD	5°	3º	7º	1º	2º	4º	6º
Sum	**10**	**14**	**14**	**18**	**17**	**15**	**12**
Results	**1°**	**3°**	**3°**	**6°**	**5°**	**4°**	**2°**

The sign (=) was used to indicate equations that presented equal scores for the calculated parameters.
Source: authors

1 CONCLUSION

The Pedotransfer Functions aim to estimate hydraulic properties of soils that are usually difficult to measure or require large financial investments to be collected. In a country like Brazil, with a large territorial extension, the development of new functions to obtain information about these characteristics is essential to reduce the cost and time to collect this data. Besides this, when used to determine the saturated volumetric moisture of the soils used in planting, these functions help in a better management of the water resources used for this practice, since the knowledge of this hydraulic parameter allows, for example, to assertively choose the best species to be planted. Avoiding the waste of water and the unusability of the soil for farming, the development of an efficient PTF also promotes sustainable agriculture.

From three soil characteristics (soil density and sand and clay fractions) obtained from the HYBRAS database, it was possible to develop a function that, when compared to six existing equations in the literature, presented a superior performance, having the value of 0.162 as the largest error between the simulated value and the measured value. Thus, the proposed pedotransfer function is effective to estimate the value of saturated moisture from the soil components.

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