

**Revista Brasileira de Engenharia Agrícola e Ambiental** ISSN 1807-1929

v.28, n.12, e278960, 2024 Brazilian Journal of Agricultural and Environmental Engineering

Campina Grande, PB – <http://www.agriambi.com.br>– <http://www.scielo.br/rbeaa>

DOI: [http://dx.doi.org/10.1590/1807-1929/agriambi.v28n1](http://dx.doi.org/10.1590/1807-1929/agriambi.v28n12e278960)2e278960

Original Article

# **Pedotransfer functions for estimating hydraulic conductivity and soil moisture in the Cerrado biome1**

Funções de pedotransferência para estimativa da condutividade hidráulica e umidade do solo no bioma Cerrado

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## *HIGHLIGHTS:*

 *Soil moistures as predictors contributed to a better performance of the pedotransfer functions (PTFs). The performance of PTFs for estimating hydraulic conductivity is hampered by the high variability of this soil property. The linear models obtained results close to the PTFs developed by more complex models in the literature.*

**ABSTRACT:** The Cerrado biome is a strategic region for Brazilian agriculture, and obtaining physical hydraulic properties is fundamental to understanding the dynamics of soil water and its impact on productivity. However, the lack and difficulty of obtaining such properties opens an opportunity to use pedotransfer functions (PTFs). In the context, the objective of the present study was to develop PTFs using multiple linear regression to estimate hydraulic conductivity of the saturated soil (Ks) and soil moisture at tensions of 0, 6, 10, 33, 100, and 1,500 kPa for the Cerrado biome. For this, two different predictor datasets were used. Dataset 1 consists of sand, silt, clay, bulk density, particle density, total porosity, microporosity, and macroporosity, and dataset 2 consists of the variables in dataset 1 plus soil moisture at field capacity (FC) and soil moisture at the permanent wilting point (PMP). Dataset 2 presented the best performance compared to Dataset 1 for estimating Ks and soil moisture, highlighting the importance of moisture in FC and PWP as predictors in the development of PTFs. However, the PTFs developed for Ks presented a low predictive capacity in all predictor datasets, unlike the soil moistures that presented high precision, with  $R<sup>2</sup>$ greater than 0.8 and errors close to zero.

**Key words:** field capacity, hydraulic conductivity, permanent wilting point, soil moisture, tropical soils

**RESUMO:** O bioma Cerrado é uma estratégica região para a agricultura brasileira e a obtenção de propriedades físico-hídricas do solo é fundamental para a compreensão da dinâmica de água no solo e o seu impacto na produtividade. Contudo, a carência e a dificuldade de obter tais propriedades abre a oportunidade de uso de funções de pedotransferência (FPTs). Sendo assim, o objetivo do presente estudo foi desenvolver FPTs utilizando regressão linear múltipla para estimativa da condutividade hidráulica do solo saturado (Ks) e da umidade do solo nas tensões de 0, 6, 10, 33, 100 e 1.500 kPa para o bioma Cerrado. Para isto, dois diferentes conjuntos de dados preditores foram utilizados. O conjunto de dados 1 consiste de areia, silte, argila, densidade do solo, densidade de partículas, porosidade total, microporosidade e macroporosidade, e o conjunto de dados 2 que consiste das variáveis do conjunto 1 mais a umidade do solo na capacidade de campo (CC) e a umidade do solo no ponto de murcha permanente (PMP). O conjunto de dados 2 apresentou o melhor desempenho quando comparado ao conjunto de dados 1, tanto para a estimativa de Ks quanto para as umidades do solo, destacando a importância das umidades na CC e PMP como preditoras no desenvolvimento de FPTs. Contudo, as FPTs desenvolvidas para Ks apresentaram uma baixa capacidade preditiva em todos os conjuntos preditores, diferentemente das umidades que apresentaram alta precisão, com R<sup>2</sup> superiores a 0,8 e erros próximos de zero.

**Palavras-chave:** capacidade de campo, condutividade hidráulica, ponto de murcha permanente, umidade do solo, solos tropicais

• Ref. 278960 – Received 27 Sept, 2023 \* Corresponding author - E-mail: mariana.f.veloso@ufv.br • Accepted 14 Jun, 2024 • Published 23 Jul, 2024 Editors: Ítalo Herbet Lucena Cavalcante & Walter Esfrain Pereira

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## **INTRODUCTION**

To establish agricultural planning strategies for Brazil's main food production region, the Cerrado biome, information on soil characteristics is essential for understanding soil water dynamics and their impacts on productivity. However, the Cerrado has a lack of and difficulty in obtaining soil properties, opening an opportunity to develop Pedotransfer Functions (PTFs).

PTFs are mathematical functions that use simple and accessible pedological data, such as contents of textural components (sand, silt, and clay), bulk density, porosity, and organic matter, to estimate soil properties obtained more difficult and costly (Pachepsky & Park, 2015). Several PTFs have been developed in recent years for estimating soil properties: bulk density (Nasta et al., 2020; Palladino et al., 2022), hydraulic conductivity (Ottoni et al., 2019; Veloso et al., 2022), water retention curve (Amorim et al., 2022; Veloso et al., 2023). However, most of the studies found in the literature were developed for temperate climate soils, which generally have different physical-hydraulic properties to tropical soils (Tomasella et al., 2000; Ottoni et al., 2019).

In Brazil, Tomasella et al. (2000) and Ottoni et al. (2019) proposed PTFs to estimate soil water retention curve and saturated hydraulic conductivity, respectively, for the country as a whole. Barros et al. (2013) developed functions for the northeast region. Kotlar et al. (2020) developed PTFs for the Amazon region. Michelon et al. (2010) developed for Rio Grande do Sul. As for the Cerrado, some studies were developed (Medrado & Lima, 2014; Veloso et al., 2022; 2023). These studies represented an advance in the physical hydraulic characterization of soils in Brazil. However, mathematical equations for estimating soil properties have not yet been published for the entire Cerrado biome. In this context, the objective of the present study was to develop PTFs using multiple linear regression to estimate hydraulic conductivity of the saturated soil (Ks) and soil moisture at tensions of 0, 6, 10, 33, 100, and 1,500 kPa for the Cerrado biome.

#### **Material and Methods**

The data used in developing the PTFs were obtained from the Veloso et al. (2022) dataset. This database is formed by soil samples from Cerrado containing data on saturated soil hydraulic conductivity (Ks), soil moisture at tensions of 0  $(\theta_0)$ , 6  $(\theta_6)$ , 10  $(\theta_{10})$ , 33  $(\theta_{33})$ , 100  $(\theta_{100})$ , and 1,500  $(\theta_{1,500})$  kPa, sand, silt, clay, bulk density, particle density, total porosity, macroporosity and, microporosity. According to Veloso et al. (2022), most of the samples in this database are classified as clayey and sandy-clay, i.e., they have considerable percentages of clay and sand in their composition.

Regarding the number of samples for the variables to be estimated, the database has 140 soil samples for the estimation of Ks, 158 samples for the estimation of soil moisture at tensions of 6 and 33 kPa, and 268 samples for the estimation of moisture at tensions of 0 (saturation moisture), 10, 100, and 1,500 kPa.

Shapiro-Wilk test was used to verify the normality of the data, analyzing the p-value  $\geq 0.05$  (5%), and those attributes that presented a tendency to non-normality were transformed using the decimal logarithm function.

All analyses and development of the PTFs were conducted using the software R (R Core Team, 2022).

The PTFs were developed considering two different datasets of predictors, dataset 1: sand, silt, clay, bulk density, particle density, total porosity, microporosity, and microporosity, and dataset 2: sand, silt, clay, bulk density, particle density, total porosity, macroporosity, microporosity, soil moisture at field capacity (10 kPa), and soil moisture at permanent wilting point (1,500 kPa).

Finally, for each variable to be estimated, different datasets of predictors were used in stepwise multiple regression models, which consists of evaluating models (Eq. 1) to identify a useful subset of predictor variables. The variables are added and removed from the model until none of these variables have the ability to increase the performance of the model.

$$
Y_{i} = \beta_{i,0} + \beta_{i,1} \cdot X_{1} + \ldots + \beta_{i,n} \cdot X_{n}
$$
 (1)

Where:

 $Y_i$  - variable to be estimated (saturated hydraulic conductivity and soil moisture at specific tensions);

 $\beta_{i,0}$  - intercept of multiple linear regression;

 $\beta_{i,1...}$   $\beta_{i,n}$  - angular coefficients linked to soil predictor variables; and,

 $X_1...X_n$  - soil predictor variables (datasets 1 and 2).

The repeated holdout method (Tanner et al., 2019) was used to validate the model. The database was divided into two independent subsets (70% for training and 30% for testing), and this process was repeated 100 times, and the average performance of these repetitions was obtained.

The statistical performance of the PTFs developed for the saturated hydraulic conductivity and soil moisture at tensions 0, 6, 10, 33, 100, and 1,500 kPa was evaluated using the statistical indexes mean error (ME) (Eq. 2), root mean square error (RMSE) (Eq. 3), and the coefficient of determination  $(R<sup>2</sup>)$  (Eq. 4).

$$
ME = \frac{1}{N} \sum_{j=1}^{N} y_j - \hat{y}_j
$$
 (2)

RMSE = 
$$
\sqrt{\frac{1}{N} \sum_{j=1}^{N} (y_j - \hat{y}_j)^2}
$$
 (3)

$$
R^{2} = \frac{\sum (\hat{y}_{j} - \overline{y}_{j})^{2}}{\sum (y_{j} - \overline{y}_{j})^{2}}
$$
(4)

Where:

 $y_j$  and  $y_j$  - are the estimated and observed values, respectively; N - the number of samples; and,

 $\Sigma(\hat{y}_j - \overline{y}_j)^2$  - is the variance explained by the model, and,  $\Sigma(\mathbf{y}_j - \overline{\mathbf{y}}_j)^2$  - is the total variance.

#### **Results and Discussion**

Table 1 contains the descriptive statistics and the Shapiro-Wilk test results of the soil properties used to estimate the Ks and soil moisture at tensions of 0, 6, 10, 33, 100, and 1,500 kPa.

Most samples have considerable percentages of sand and clay (Table 1). Clay textured soils generally have a higher water storage capacity, and the average clay content equal to 42.16% observed in the soils used for the development of PTFs indicates that, in general, the soils of the Cerrado biome have a good water storage capacity. In addition, clayey soils, especially well-structured soils such as Oxisols, a soil class considered predominant in the Cerrado (Ab'Sáber, 1983), show a behavior contrary to generalizations of soil hydraulic processes, which is one of the reasons for the low accuracy of PTFs developed for temperate regions when applied in tropical areas.

Particle density was the variable that presented the lowest coefficient of variation with 3.64%, which is a soil property that does not oscillate much in its values (Weil & Brady, 2016). On the other hand, Ks showed the highest coefficient of variation, with 138.49%, indicating high inherent variability of this physical hydraulic property (Sarki et al., 2014).

Regarding the Shapiro-Wilk test, the results show that the attributes saturated hydraulic conductivity, sand, silt, clay, bulk density, particle density, total porosity, microporosity, and macroporosity present a tendency towards non-normality of the distribution of data; therefore, these variables were submitted to logarithmic transformation. Thus, Table 2 presents the correlation coefficient (r) obtained after transforming the data to evaluate the correlation between the estimated variables, saturated hydraulic conductivity, and moisture of the soil at different tensions with the predictor variables of the soil.

The highest correlation values for saturated hydraulic conductivity were with the variables bulk density (-0.50), total porosity (0.44), macroporosity (0.39), and soil moisture at a tension of 1,500 kPa (-0.42). In other words, the higher the Ks values, the higher the values of total porosity and macroporosity. Also, the Ks values decrease as the bulk density and soil moisture in the PWP increase. This decrease may be associated with the compaction process and the loss of water **Table 2.** Correlation coefficient (r) between the predictor variables and the saturated hydraulic conductivity and soil moisture in different matrix potentials of the samples used to generate the pedotransfer functions for the Cerrado biome



Ks - Saturated hydraulic conductivity of soil (mm h<sup>-1</sup>);  $\theta_0$ ,  $\theta_8$ ,  $\theta_{10}$ ,  $\theta_{33}$ ,  $\theta_{100}$ , and  $\theta_{1,500}$  - Soil moisture at tensions of 0, 6, 10, 33, 100, and 1,500 kPa, respectively; Bd - Bulk density (g cm-3); Pd - Particle density (g cm-3); Tp - Total porosity (%); Micro - Microporosity (%); Macro - Macroporosity (%)

in the soil, where macropores empty and turn into micropores, and the hydraulic conductivity is more determined by the matrix potential (Zhang et al., 2019).

On the other hand, water retention, in general, presented the best correlations with the other moisture contents and the structural attributes (microporosity and microporosity) and a moderate correlation with the textural attributes (sand and clay). According to Pozdnyakov et al. (2006), capillary forces are more present at higher potentials, with a greater influence from structural properties. On the other hand, at lower potentials, soil adsorption processes are more active, with a greater influence from textural and soil attributes (specific surface of the particles). However, as can be seen in Table 2, at the lowest potentials (33, 100, and 1,500 kPa), the structural variables microporosity and macroporosity showed higher correlation values than the textural variables, and this can be explained by the fact that soils from the Cerrado region are mostly classified as Oxisols, which are more structured soils.

Regarding the textural attributes, the contents of sand presented a negative correlation, and clay presented a positive correlation with water retention due to the opposite behavior of these variables, a fact also identified in the work of Michelon et al. (2010) and Barros et al. (2013).





Bd - Bulk density; Pd - Particle density; Tp - Total porosity; Micro - Microporosity; Macro - Macroporosity; Ks - Saturated hydraulic conductivity;  $\theta_{o}$ ,  $\theta_{e}$ ,  $\theta_{10}, \theta_{13}, \theta_{100}, \theta_{13}, \theta_{100},$  and  $\theta_{1,500}$  - So moisture at tensions of 0, 6, 10, 33, 100, and 1,500 kPa, respectively; CV - Coefficient of variation; W - Shapiro-Wilk normality test value; P(\*) - Tendency to normality. p-value ≥ 0.05

The PTFs developed to estimate Ks using predictor datasets 1 and 2 did not provide an adequate fit to the data. The equations obtained to estimate the saturated hydraulic conductivity and their respective  $R^2$  are shown in Table 3.

The RMSE values were 0.584 and 0.558 mm h-1 for datasets 1 and 2, respectively. The ME values were close to zero, equal to -0.01 (dataset 1) and 0.01 (dataset 2). Veloso et al. (2022) found it difficult to develop PTFs for estimating Ks in the Cerrado biome, even when using more complex models, such as machine learning algorithms. The authors used the same variables as in datasets 1 and 2 and obtained R² values between 0.16 and 0.53 and RMSE values between 32 and 44 mm h-1. This difficulty in developing PTF for estimating Ks in the Cerrado biome may be associated with the high variability of this property, as shown by the high CV value in Table 1.

Most PTFs for Ks estimation were developed using granulometric variables and/or bulk density, with the use of soil moisture as an uncommon predictor (Tóth et al., 2015; Ottoni et al., 2019). However, incorporating structural variables to estimate Ks can better explain the property. This fact can be observed only in the result presented from the dataset 2 predictor with the incorporation of soil moisture.

The bulk density was the only variable that was present in the composition of the PTFs using the datasets of predictors 1 and 2, corroborating the results presented in Table 2, which shows a higher correlation of Ks with the density of the soil. Furthermore, it can be verified that the macroporosity and total porosity variables, which presented positive correlations with Ks, were not present in the composition of the equations. In the PTF of dataset 1, soil moisture was added to the PWP in the composition of the equation, an attribute of negative correlation with Ks along with Bd.

Ottoni et al. (2019) highlighted that the performance of PTFs is not only influenced by the correlation between the estimated property with the predictor variables, but the database used for training and testing these functions also strongly contributes to performance. Therefore, the low sample quantity used to develop PTFs to estimate Ks may have influenced its low predictive capacity.

About the PTFs for estimating soil moisture, only the PTFs for soil moisture at tensions of 33 and 1,500 kPa using predictor dataset 1 did not show an adequate fit with the data (Figures 1I, 1J). For the other PTFs, Figure 1 shows the graphs of estimated soil moisture versus observed soil moisture at tensions of 0 (Figures 1A, 1B), 6 (Figures 1C, 1D), 10 (Figure 1E, 1F), 33 (Figure 1I), 100 (Figures 1G, 1H), and 1,500 (Figure 1J) kPa, and their respective statistical indexes R², RMSE, and ME obtained by datasets 1 and 2.

The best estimate for soil moisture at tensions of 0, 6, 10, 33, 100, and 1,500 kPa was observed using the predictor dataset 2 with R² values above 0.8 for all moistures, except for

moisture at the tension 0 kPa (Figure 1B). The RMSE and ME values were close to zero in all PTFs, with variations between 0.02 and 0.06  $\text{m}^3$  m<sup>-3</sup> and -0.01 and 0.01 m<sup>3</sup> m<sup>-3</sup>, respectively, indicating a low magnitude of the errors in the soil moisture estimates at the tensions evaluated. In a study conducted by Tomasella et al. (2000), RMSE values from 0.032 to 0.427 m3 m<sup>-3</sup> were obtained for tropical soils, a variation close to the results obtained in this study for the Cerrado biome.

Michelon et al. (2010) also obtained RMSE and ME values close to zero for soil moisture at tensions of 0, 1, 33, 100, 500, and 1,500 kPa, and  $R<sup>2</sup>$  values above 0.7, using the variables corresponding to the dataset 1 to develop PTFs for the Rio Grande do Sul state. Compared to the study conducted for the Cerrado biome using machine learning algorithms, Veloso et al. (2022) obtained excellent results in estimating soil moisture at different tensions, with the best results using the same variables as dataset 2, with  $R<sup>2</sup>$  values varying between 0.79 and 0.95 and RMSE values between  $-0.01$  and  $0.02$  m<sup>3</sup> m<sup>-3</sup>. Despite the simplicity of multiple linear regression compared to the machine learning (ML) algorithms used by Veloso et al. (2022), the FPTs developed in this study showed  $R<sup>2</sup>$  values relatively close to those developed by ML.

Now, the improvement in the explanation of the variables when the FC and PWP soil moisture data were incorporated into the estimation of another soil water content data allowed for a better fit of the models, which can be seen from the increase in the  $R<sup>2</sup>$  values from the models in dataset 1 to the models in dataset 2.

The PTFs developed for estimating soil moisture at tensions of 0, 6, 10, 33, 100, and 1,500 kPa using the predictor datasets 1 and 2 are shown in Table 4.

In general, the PTFs developed for both the highest and the lowest soil tensions presented textural variables in their compositions, mainly clay. The structural variables, microporosity, macroporosity, and moisture in the FC and PWP were present in the PTFs when incorporated into datasets 1 and 2. These results agree with Table 2, highlighting a higher correlation between these structural attributes and water retention.

The PTFs developed with dataset 2 showed at least one of the soil moistures in their composition in all equations. Many PTFs published in the literature do not use soil moisture contents as predictors. In one of the few studies using soil moisture content to estimate FC and PWP, Gunarathna et al. (2019) and Veloso et al. (2022; 2023) developed PTFs using machine learning algorithms and obtained better performances when incorporating soil moisture as predictors in the model. Therefore, using these variables can contribute to the estimation when the soil moisture data in the FC and/or PWP are available, most frequently obtained in the laboratory.

**Table 3.** Pedotransfer functions (PTFs) for estimating the saturated hydraulic conductivity of soil in the Cerrado biome



Ks - Saturated hydraulic conductivity (mm h<sup>-1</sup>);  $\theta_0$ <br>R<sup>2</sup> - Coefficient of determination n h<sup>-1</sup>);  $\theta_0$ ,  $\theta_6$ ,  $\theta_{10}$ ,  $\theta_{33}$ ,  $\theta_{100}$  and  $\theta_{1,500}$ . Soil moisture at tensions of 0, 6, 10, 33, 100, and 1,500 kPa, respectively; Bd - Bulk density (g cm<sup>-3</sup>);



RMSE – Root Mean Square Error; ME – Mean Error; R² - Coefficient of determination. Figure 1. Predicted soil moisture versus observed soil moisture at tensions of 0 kPa (A, B), 6 kPa (C, D), 10 kPa (E, F), 33 kPa (I), 100 kPa (G, H), and 1,500 kPa (J) obtained by predictor datasets 1 and 2



Dalasel <b>Predictor</b>	PTF	R <sup>2</sup>
	$\theta_0 = 0.3174383 - 0.0730122$ (log(Sand)) - 1.0636051(log(Bd)) + 1.0621988(log(Pd)) - 0.022102(log(macro))	0.71
	$\theta_6 = -1.0186139 + 0.248967(\log(Clay)) + 0.6977942(\log(Pol)) + 0.4748349(\log(Tp)) - 0.1003896(\log(maxro))$	0.65
	$\theta_{10} = -0.4836716 + 0.1764649$ (log(Clay)) + 0.1785483(log(Bd)) + 0.3710038(log(micro)) – 0.0504698(log(macro))	0.64
	$\theta_{33} = -0.50243206 + 0.3031745(\log(Clay)) + 1.02206019(\log(Bd)) - 0.08008585(\log(macro))$	0.56
	$\theta_{100} = -0.56801394 + 0.19508774(log (Clay)) + 0.6912217(log (Pd)) + 0.21932143(log (micro)) - 0.06917081(log (macro))$	0.64
	$\theta_{1,500} = -0.24688953 + 0.04792146(log(Silt)) + 0.22503525(log(Clay)) + 0.4445548(log(Pd)) - 0.08125156(log(macro))$	0.58
C.	$\theta_0 = 0.1814579 - 1.088485(\log(Bd)) + 0.8529062(\log(Bd)) + 0.3163872\theta_{1500}$	0.77
	$\theta_6 = -0.07549893 + 0.06060497$ (log(Clay)) + 1.19910227 $\theta_{10}$ – 0.27752582 $\theta_{1500}$	0.89
	$\theta_{10} = -0.19465425 - 0.03766904(log(Silt)) + 0.2389363(log(micro)) + 0.79487795\theta_{1500}$	0.85
	$\theta_{33} = 0.04195487 + 0.23929856\theta_{10} + 0.75331832\theta_{1500}$	0.95
	$\theta_{100} = -0.1098622 + 0.2690601(log(Pd)) + 0.3614433\theta_{10} + 0.6516879\theta_{1500}$	0.95
	$\theta_{1500} = -0.02612024 + 0.0414105$ (log(Silt)) + 0.06193916(log(Clav)) - 0.08934998(log(micro)) + 0.83206566 $\theta_{10}$	0.82

0<sub>0</sub>, 0<sub>6</sub>, 0<sub>10</sub>, 0<sub>3</sub>, 0<sub>100</sub>, and 0<sub>1500</sub> - Soil moisture at tensions of 0, 6, 10, 33, 100, and 1,500 kPa, respectively; Bd - Bulk density; Pd - Particle density; Tp - Total porosity; Micro - Microporosity;<br>Macro - Macr

## **Conclusions**

1. In general, the PTFs constituted by FC, PWP, granulometric, and structural attributes (dataset 2) presented the best results in the estimates of the soil moisture at the tensions of 0, 6, 10, 33, 100, and 1,500 kPa, when compared to PTFs constituted only by granulometric and structural attributes (dataset 1).

2. The PTFs for estimating hydraulic conductivity did not provide accurate results.

3. The soil moisture at tensions of 0, 6, 10, 33, 100, and 1,500 kPa can be accurately estimated from the PTFs with the granulometric, structural, FC, and PWP attributes.

**Contribution of authors:** M. F. Veloso worked on research, data acquisition, data analysis, implementation of the computational simulations, and writing of the manuscript. L. N. Rodrigues served as research advisor and worked on the conceptualization of the problem, literature review, data acquisition, improvements and corrections to the manuscript. E. I. Fernandes Filho advised and worked on data analysis, and corrections and improvements to the simulation models.

**Supplementary documents**: There are no supplementary sources.

**Financing statement:** The study was funded by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES – Finance Code 001).

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