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USE OF PEDOTRANSFER EQUATIONS (PTF) TO ESTIMATE SOIL DENSITY IN THE HYDROGRAPHIC BASINS OF THE AMAMBAI, IGUATEMI AND IVINHEMA RIVERS IN THE STATE OF MATO GROSSO DO SUL

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ABSTRACT

Theoretical framework: Bulk density (Bd) is a physical property of soil used as an indicator of soil compaction, influencing root growth and density, water movement and retention in the soil, it is an essential characteristic for assessments of carbon stocks or other nutrients in the soil.

Objective: This studyevaluates the accuracy and selects pedotransfer functions (PTFs) for Bd estimates for soils in the Amambai, Iguatemi, and Ivinhema River basins in Mato Grosso do Sul - MS.

Method: Estimates of Bd values of the samples were made using eleven PTFs-Bd that were calibrated to estimate Bd for Brazilian soils. The accuracy of PTFs-Bd predictions is evaluated based on the lowers root mean square error (RMSE) and the highers coefficient of determination (R^2).

Results and conclusion: Among the eleven analyzed PTFs-Bd, the most accurate ones were PTFs- Ds 1, 2, 3, and 4 by Huf dos Reis et al. (2024) and the one by Tomasella and Hodnett (1998). PTF-Bd 3, which uses fine and coarse sand and clay as predictors, showed the highest accuracy for the total dataset (88 samples). PTF-Bd 5 obtained better accuracy in estimating Bd in Latossolos Vermelhos, Argissolos Vermelho Amerelos, and Neossolos Quartzarênicos.

Research implications: Identifying the best PTFs for estimating Bd for the study area's soils will facilitate other research as carbon stocks estimation and use of hydrophysical PTFs that use Bd as predictor.

Originality/Value: PTFs for estimating Bd for soils in the state of MS have not yet been developed, highlighting the need to evaluate and indicate between existing PTFs the more accurate.

Keywords: Pedotransfer Function, Bulk Density, Soil Class, Textural Class, Land Use.

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USO DE EQUAÇÕES DE PEDOTRANSFERÊNCIA (PTF) PARA ESTIMATIVA DA DENSIDADE DO SOLO NAS BACIAS HIDROGRÁFICAS DOS RIOS AMAMBAI, IGUATEMI E IVINHEMA NO ESTADO DO MATO GROSSO DO SUL

RESUMO

Referencial teórico: A densidade do solo (Ds) é uma propriedade física utilizada como indicador do grau de compactação do solo, influenciando o crescimento e a densidade de raízes, a movimentação e a retenção de água no solo. É uma propriedade indispensável para avaliações de estoques de carbono e de nutrientes no solo.

Objetivo: Este artigo avalia a acurácia e seleciona funções de pedotransferência (PTFs) para estimativas de Ds (PTF-Ds) para os solos das bacias dos Rios Amambai, Iguatemi e Ivinhema no Mato Grosso do Sul - MS.

Método: Foram feitas estimativas dos valores de Ds de 88 amostras por onze PTFs-Ds que foram calibradas para estimar Ds para solos do Brasil. A avaliação da acurácia das predições das PTFs-Ds baseia-se nos índices: menores valores da raiz do erro quadrático médio (RMSE) e maiores valores do coeficiente de determinação (R^2).

Resultados e conclusão: As PTFs-Ds mais acuradas dentre as onze analisadas foram as PTFs-Ds 1, 2, 3 e 4 de Huf dos Reis et al. (2024) e a PTF-Ds 5 de Tomasella e Hodnett (1998). A PTF-Ds 3 que utiliza como preditores areia fina e grossa e argila apresentou maior acurácia para o conjunto total de dados (88 amostras). A PTF-Ds 5 obteve melhor acurácia ao estimar Ds em Latossolos Vermelhos, Argissolos Vermelho Amarelos e Neossolos Quartizarênicos.

Implicações da pesquisa: Encontrar as melhores PTFs para estimativa da Ds para os solos da área de estudo, permitirá cálculos de estoques de carbono e do uso de outras PTFs que necessitam dessa propriedade.

Originalidade/valor: PTFs para estimativa de Ds para os solos do estado do MS ainda não foram desenvolvidas, então há necessidade em indicar PTFs já existentes para o uso na região de estudo.

Palavras-chave: Função de Pedotransferência, Densidade do Solo, Classe de Solo, Classe Textural, Uso da Terra.

1 INTRODUCTION / THEORETICAL REFERENCE

Soil density (Ds) is the ratio of the mass of a dry soil sample (in g) to its volume (solids plus pores, in cm³) (Hillel, 1998).

It is considered one of the fundamental physical properties of soil. Indicator of the degree of soil compaction, influencing root growth and density, soil movement and water retention, is an indispensable characteristic for assessing carbon stocks or other nutrients in the soil (Reichardt and Timm, 2004; De Vos et al., 2005).

The volumetric cylinder method is the one most used for Ds measurements. It consists of the collection of a sample of unformed soil by insertion into the soil of a volumetric cylinder of known volume for the determination of a sample of known volume and mass. The samples are dried in an oven at 105 °C and then weighed to obtain the dry mass of the soil. Ds is then calculated by dividing the mass (g) by the volume of the cylinder, in cm³ (Teixeira et al., 2017).

Another method of estimating Ds is the use of Pedotransfer Functions (PTFs), which has been used by soil scientists to overcome the constraints associated with direct measurements (Obidike-Ugwu et al., 2023).

The *PedoTransferFunction* (PTF) is a predictive statistical tool based on the most widely available physical and chemical soil properties and measurements (Bouma, 1989).

These PTFs were developed to estimate Ds from a specific data set such as granulometry (sand, silt and clay fraction contents) organic carbon (CO) content, pH, sum of cations (Benites et al., 2007, Alexander, 1980; Manrique and Jones, 1991; Kaur et al., 2002; Souza et al., 2016; Nanko et al., 2014), also class data land use and soil depth (Palladino et al. 2022).

PTFs for estimates of Ds (PTFs-Ds) have been elaborated both for regional estimates (Tomasella and Hodnett., 1998; Bernoux, et al., 1998; de Souza, et al., 2016; Barros, et al., 2015), as well as national (Benites et al., 2007; Huf dos Reis, 2024) and global (Rawls, 1983; Han, et al., 2012; Al-Qinna and Jaber, 2013; Nanko et al., 2014; Sevastas et al., 2018; Palladino et al., 2022; Obidike-Ugwu, 2023). However, the use of PTFs in different regions from which they were calibrated must have their accuracy assessed beforehand (Kaur et al., 2002; McBratney et al., 2002).

The objective of this study is to evaluate the accuracy, select and indicate PTFs for estimates of Ds for the soils of the Amambai, Iguatemi and Ivinhema rivers in Mato Grosso do Sul.

Specific objectives:

1. Estimate the density of the soil through eleven pedotransfer functions.
2. Assess the accuracy of soil density predictions in the different basins.
3. Indicate the most accurate PTFs for the study region, depending on the availability of predictor parameters for the Amambai, Iguatemi and Ivinhema basins.

2 METHOD

2.1 Field of Study

The study covered a search for data on soil density and soil parameters in the areas of the basins of the Amambai, Iguatemi and Ivinhema Rivers in the state of Mato Grosso do Sul, which total an area of 64,000 km² in extension covering 37 municipalities (Figure 1). The climate of the study region according to the Köppen classification is the subtype Cfa - humid subtropical (Alvares et al., 2013).

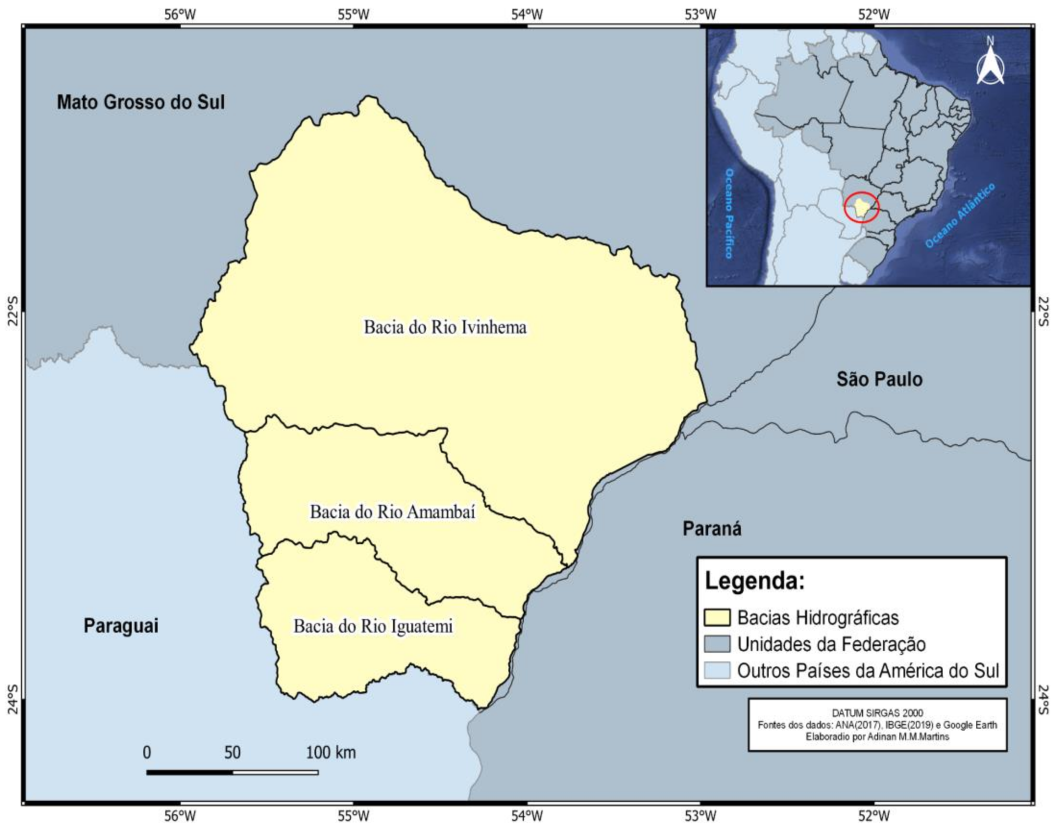

Figure 1: Location map of the basins of the Ivinhema, Amambaí and Iguatemi Rivers.
Source: ANA, 2017; IBGE-BDIA, 2019 and Google Earth, adapted by Martins, A. M. M.

2.2 Data Selection and Description

A database (BD-MS_Ds) was organized with soil density data (Ds) from the three basins of the study area, which were obtained in published works. BD-MS_Ds totals 88 observed Ds data, including information on clay, silt, fine and coarse sand and organic carbon (CO) contents.

BD-MS_Ds also has location data, such as municipality, microbasin, coordinates and elevation. In addition to soil class, land use systems, depth and textural class.

The soil class and textural class data were harmonized according to the Brazilian Soil Classification System (dos Santos et al., 2023) and the land use systems by the caption of MapBiomas Collection 7 (2023).

2.3 Selection of PTFs for Ds Estimates (PTF-Ds)

Estimates of the Ds values of the samples were made by eleven PTFs-Ds that were calibrated to estimate Ds for soils in Brazil (Table 1). Only samples that were within the range of particle and carbon content values for which the PTF-Ds were developed (function domain) were considered. These PTF-Ds and the necessary predictors of them are described in Table 1 and their domains in Table 2.

Table 1. Pedotransfer functions of Huf dos Reis et al (2024), Tomasella and Hodnett (1998), Bernoux et al (1998) and Benites et al (2007), their predictors and number of samples used to develop each PTF-Ds.

Functions	References	Predictors	PTF	NO
		%		
PTF-Ds 1	Huf dos Reis et al, 2024 - 1	*Sand, Clay*	$Ds = 1.286 + 3.208 \times 10^{-3}(Sand) - 2.013 \times 10^{-3}(Clay)$	3,050
PTF-Ds 2	Huf dos Reis et al, 2024 - 2	*Sand, Clay, CO*	$Ds = 1.358 + 2.79 \times 10^{-3}(Sand) - 2.328 \times 10^{-3}(Clay) - 0.052(CO)$	2,827
PTF-Ds 3	Huf dos Reis et al, 2024 - 3	*Sand f, Sand g, Clay*	$Ds = 1.198 + 2.971 \times 10^{-3}(Sand\ f) + 4.472 \times 10^{-3}(Sand\ g) - 8.706 \times 10^{-4}(Clay)$	1,081
PTF-Ds 4	Huf dos Reis et al, 2024 - 4	*Sand f, Sand g, Clay, CO*	$Ds = 1.243 + 2.983 \times 10^{-3}(Sand\ f) + 4.187 \times 10^{-3}(Sand\ g) - 5.793 \times 10^{-4}(Clay) - 6.208 \times 10^{-2}(CO)$	990
PTF-Ds 5	Tomasella and Hodnett, 1998	*Clay, Silt, CO*	$Ds = 1{,}578 - 0{,}058(CO) - 0{,}006(Silt) - 0{,}004(Clay)$	2,827
PTF-Ds 6	Bernoux et al, 1998 - 1	*Clay*	$Ds = 1{,}352 - 0{,}0045(Clay)$	2,955
PTF-Ds 7	Bernoux et al, 1998 - 2	*Clay, CO*	$Ds = 1{,}398 - 0{,}0047(Clay) - 0{,}042(CO)$	2,711
PTF-Ds 8	Benites et al, 2007 - 1	*Clay*	$Ds = 1{,}5224 - 0{,}0005(Clay)$	3,050
PTF-Ds 9	Benites et al, 2007 - 2	*Clay, CO*	$Ds = 1{,}5688 - 0{,}0005(Clay) - 0{,}009(CO)$	2,804
PTF-Ds 10	Benites et al, 2007 - 3	*Clay, CO*	$Ds = 1{,}554 - 0{,}0004(Clay) - 0{,}01(CO)$	423
PTF-Ds 11	Benites et al, 2007 - 4	*Clay, CO*	$Ds = 1{,}567 - 0{,}0005(Clay) - 0{,}006(CO)$	345

N° - number of samples; Sand f - fine sand; Sand g - thick sand; CO - organic carbon;
Source: authors.

Table 2. Predictor domains for pedotransfer functions of Huf dos Reis et al. (2024), Tomasella and Hodnett (1998), Bernoux et al (1998) and Benites et al (2007).

Functions	References	Clay	Silt	Sand f	Sand g	Total Sand	CO
				%			
PTF-Ds 1	Huf dos Reis et al, 2024 - 1	*0-96*	THE	THE	THE	0-98,8	THE
PTF-Ds 2	Huf dos Reis et al, 2024 - 2	*0-96*	THE	THE	THE	0-98,8	0-9,8
PTF-Ds 3	Huf dos Reis et al, 2024 - 3	*0-96*	THE	0-97,2	0-97	THE	THE
PTF-Ds 4	Huf dos Reis et al, 2024 - 4	*0-96*	THE	0-97,2	0-97	THE	0-9,8
PTF-Ds 5	Tomasella and Hodnett, 1998	*0-100*	0-71	THE	THE	THE	THE
PTF-Ds 6	Bernoux et al, 1998 - 1	*3,9-90,75*	THE	THE	THE	THE	THE
PTF-Ds 7	Bernoux et al, 1998 - 2	*3,9-90,75*	THE	THE	THE	THE	0,04-12,16
PTF-Ds 8	Benites et al, 2007 - 1	*0-96*	THE	THE	THE	THE	0,03-20,6
PTF-Ds 9	Benites et al, 2007 - 2	*0-96*	THE	THE	THE	THE	0,03-20,6
PTF-Ds 10	Benites et al, 2007 - 3	*0-96*	THE	THE	THE	THE	0,03-20,6
PTF-Ds 11	Benites et al, 2007 - 4	*0-96*	THE	THE	THE	THE	0,03-20,6

Sand f - fine sand; Sand g - coarse sand; CO - organic carbon; NA - not applicable;
Source: authors.

The evaluation of the accuracy of the predictions of PTFs-Ds was based on the indices: *Root Mean Square Error* root (*RMSE*) estimated using Equation 1 and the coefficient of determination (R^2) which is based on the covariance between the observed and predicted Ds values (Equation 2)

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=n}^{N}(yi - \hat{yi})^2} \qquad \text{Equation 1}$$

$$R^2 = 1 - \frac{\sum_{i=1}^{N}(yi - \hat{yi})^2}{\sum_{i=1}^{N}\left(yi - \underline{yi}\right)^2} \qquad \text{Equation 2}$$

Where:

$\hat{yi}$ *é a estimativa do valor*, $\underline{yi}$ *é a média dos valores observados*, *yi é o valor observad*

The best average accuracy of prediction among the different PTFs-Ds tested is indicated by higher R^2 values and lower RMSE values. The accuracy of the estimates of PTF-Ds was estimated for the total data set (88 samples) and grouped by soil class, texture class and land use system.

1:1 correlation graph between predicted and observed Ds data were made for the five PTF-Ds that presented the smallest RMSE (Huf dos Reis et al. 2024).

Graphical analysis of waste dispersion *versus* predicted values for soil classes, textural classes and land use systems.

3 RESULTS AND DISCUSSION

The data of Ds available in (BD-MS_Ds) comprises four soil classes according to the Brazilian Soil Classification System (dos Santos et al., 2023). The soil class with the highest number of data is the Latossolo Vermelho, with 75 samples. The other classes that have data of Ds in the region studied are the Plintossolos Argilúvicos, the Argissolos Vermelho Amarelos and the Neossolo Quartizarênico with 5, 4 and 4 samples each respectively (Table 4). The 88 samples available are distributed in eight textural classes (Table 5). The very clayey texture is more frequent with 34 samples, and only one sample has a Clay loam texture.

Five land use systems were identified, with the systems classified as forest formation and pasture, the ones that presented the largest numbers of samples with 35 and 27 samples, respectively. The systems that were not possible to be classified are called Mosaic of uses with five samples, this system of land use was not considered in the analyzes of accuracy for systems of use.

Ds data ranged from 0.91 to 1.80 g cm^{-3}, averaging 1.33 g cm^{-3} (Table 3).

Table 3 shows the ranges of values (maximum-minimum) of clay, silt, fine sand, coarse sand and organic carbon content of the Ds samples that were used as predictors for the Ds estimates, with these ranges it is possible to verify whether they meet the domain of predictor parameters with which the equations were adjusted (Table 2).

Table 3. Descriptive statistics of soil density (Ds), particle size fractions, and organic carbon (CO) contents for the soil database (BD-MS_Ds) of Mato Grosso do Sul.

Descriptive Statistics	Ds	Clay	Silt	Total sand	Fine sand	Coarse sand	CO
	g/kg			— %—			
Maximum	1.80	77	34	93	56	51	2.92
Minimum	0.91	3.	3.	11	5	2.	0.10
Medium	1.32	41	12	48	26	21	0.76
Median	1.40	54	11	27	16	10	0.71
Standard deviation	0.23	26	7	29	15	16	0.73

Source: authors.

The best accuracy among the eleven PTF-Ds evaluated is indicated by the lowest RMSE values and highest R^2 values (Table 4).

Among the PTF-Ds evaluated, the proposal by Benites et al. (2007), identified as PTF-Ds 11, showed the highest RMSE, reaching a value of 0.290. On the other hand, PTF-Ds 3, also authored by Benites et al. (2007) and identified as PTF-Ds 10, showed the lowest R^2, with a value of 0.299. These results suggest that these functions exhibited the smallest accuracy among the equations analyzed.

The finding of a low value of R^2, as observed in the proposals of Benites et al. (2007), which was in the order of 0.11, was also corroborated by Souza et al. (2016). The latter study estimated the soil density values (Ds) for 242 soil samples in the Doce River basin, located in Minas Gerais. The authors attributed the low accuracy of PTF-Ds to the high variability present in the data set used for the development of these equations.

The PTFs-Ds 1, 2, 3 and 4 of Huf dos Reis et al. (2024) and the PTF-Ds 5 of Tomasella and Hodnett (1998) obtained the best indices (low RMSE and high R^2) among the eleven PTFs tested.

Table 4. Estimates of the accuracy of predictions (Root Mean Square Error - RMSE and coefficient of determination R^2) of soil density for the eleven PTFs initially evaluated from the soils studied in the basins of the Amambai, Iguatemi and Ivinhema Rivers in Mato Grosso do Sul.

Functions	References	RMSE	R^2
PTF-Ds 1	Huf dos Reis et al, 2024 - 1	**0.1677**	**0.338**
PTF-Ds 2	Huf dos Reis et al, 2024 - 2	**0.1707**	**0.333**
PTF-Ds 3	Huf dos Reis et al, 2024 - 3	**0.1635**	**0.336**
PTF-Ds 4	Huf dos Reis et al, 2024 - 4	**0.1671**	**0.320**
PTF-Ds 5	Tomasella and Hodnett, 1998	**0.1685**	**0.318**
PTF-Ds 6	Bernoux et al, 1998 - 1	0.2246	0.335
PTF-Ds 7	Bernoux et al, 1998 - 2	0.2022	0.336
PTF-Ds 8	Benites et al, 2007 - 1	0.2621	0.335
PTF-Ds 9	Benites et al, 2007 - 2	0.2895	0.317
PTF-Ds 10	Benites et al, 2007 - 3	0.2818	0.299
PTF-Ds 11	Benites et al, 2007 - 4	0.2902	0.330

Source: authors.

Low levels of Ds are usually found in soils with high levels of organic matter and/or clay, especially clay soils and very well-structured clay soils such as Latossolos and Argissolos under the original vegetation. The lowest value of Ds 0.91 g cm^{-3} found in this study, corroborating this affirmative, was determined in a very clay, Latossolo Vermelho in the study by Camargo and Freitas, 1971.

High Ds values are found in sandy soils (e. g. Neossolos Quartizarêncos and Espodossolos) (Huf dos Reis et al, 2024; Ottoni et al., 2018). In the database (BD-MS_Ds) there are no samples of Spodossoils, despite the occurrence of this soil in the studied region (SEPLAN, 1988). The highest value of Ds (1.80 g cm^{-3}) was found in an Plintossolo Argilúvico soil with Sandy clay loam textural class, under pasture (Camargo and Freitas, 1971).

Graphical analysis of the residues between observed and predicted Ds data for Huf dos Reis, et al (2024) and Tomasella and Hodnett (1998) presented in Figure 2, shows that the largest residues (underestimations of order 0.4 g cm^{-3}) were found in six samples with the highest Ds values, ranging from 1.66 to 1.80 g cm^{-3} (Figure 2). This data comes from areas with Latossolo Vermelho and Plintossolo Argilúvico, with system of use of agriculture and pasture (Sobrinho et al. 2003; Camargo e Freitas, 1971). These use systems may have caused soil compaction due to inadequate management systems, as observed by Santana et al. (2018) in Argissolos Vermelho Amarelos in northeastern Brazil. The textural class of these samples is very clayey and clayey, which generally have low Ds values in their original condition, however soils of these textural classes are susceptible to compaction and increased Ds indices. These facts reinforce that the specificity of the data set used for estimating Ds, can change the results of LBTs and the great challenge for an accurate LBT-Ds is the inclusion of a structural parameter, which ~~allows~~ differentiating soils with similar granulometry and carbon contents, but with different structures or degrees of compaction.

The PTFs-Ds of Huf et al. (2024) were developed in a hierarchical system with the inclusion of different predictor parameters of Ds (Table 1). The inclusion of more predictor parameters does not necessarily improve accuracy indices (MMR. and R^2) (Table 4).

In this study, PTFs-Ds 2 and 3 obtained good acuracies, with MMR. close to those found by PTFs-Ds 2 and 3 of Huf dos Reis et al. (0.16 g cm^{-3}) (Table 4 and Figure 2).

PTF-Ds 1 by Huf dos Reis et al., (2024) which used only clay and sand data, showed the RMSE value of 0.167 g cm^{-3}. PTF-Ds 2, which uses clay, sand, and CO as predictors, increased the MMR. to 0.170 g cm^{-3}. PTF-Ds 3 that does not use CO but fractionates the total sand into fine and coarse sand, reduced the value of MMR. to 0.163 g cm^{-3}, being the one that presented better accuracy among the four PTF-Ds proposed by Huf et al., (2024). The PTF 4 predictors of clay, fine sand, coarse sand and CO in this study presented a value of 0.167 g cm^{-3}, showing that not always the addition of more predictor variables will increase accuracy.

Tomasella and Hodnett developed PTF-Ds 5 (Table 1) from the results of Ds evaluated in Amazon soils, they found a value of R^2 of 0.60 g cm^{-3}. Huf dos Reis et al (2024), using data from Ds across Brazil estimated an MMR. of 0.20 and R^2 of 0.37 g cm^{-3} for PTF-Ds 5. Boschi et al. (2018) evaluated a set with 884 soil samples for all Brazilian biomes and found that PTF-Ds 5 presented a value of R^2 of 0.40 and RMSE of 0.19 g cm^{-3}. Benites et al. (2007) using PTF-Ds 5 from Tomasella and Hodnett (1998) found an MMR. of 0.28 g cm^{-3} in a study with 613 samples. The present study also found good accuracy for the PTF-Ds 5 of Tomasella and Hodnett (1998), which obtained an RMSE value of 0.17 g cm^{-3} the third lowest value among the PTF-Ds tested (Table 4 and Figure 2).

According to De Vos et al. (2005), a PTF-Ds exhibits satisfactory accuracy when the MMR. is between 0.12 and 0.25 g cm^{-3}. Following this criterion, the PTFs-Ds 1,2,3,4 and 5 showed good accuracy for the soils of Mato Grosso do Sul when analyzed in a global manner, without distinction of textural class, soil class and by land use.

Figure 3 shows the results of the 1:1 dispersion charts and correlation data (R^2) between observed and predicted values of Ds for PTFs-Ds 1, 2, 3, 4 and 5, classified also in soil classes, textural class and land use system. It is observed that Ds tends to be overestimated Neossolos Quartzarênicos, mainly in systems of use as pasture (Figure 3). The Ds values of the Plintossolo Argilúvico were underestimated (Figure 2).

They were made from the RMSE by soil class, textural class and land use, presented in Tables 5, 6 and 7 (Figures 2 and 3). The MMR.s reduced their values when classified by these criteria, less for the soil class Plintosolo Argilúvico (Table 5), textural class Sandy loam and very clay (Table 6) and land use system Agriculture (Table 7).

PTF-Ds 3 developed by Huf dos Reis et al. (2024) obtained the best accuracy among the five models when analyzing all data from Mato Grosso do Sul together (RMSE = 0.163 g cm^{-3}), but if the data set is analyzed separately, by the use systems, soil class and textural class, the PTFs-Ds present different accuracy.

The PTF-Ds 5 of Tomasella and Hodnett (1998), which obtained the fourth best accuracy with all data, was the one that showed the greatest improvement in the MMR values when the data were analyzed separately. Considering the most representative data (largest number of samples), PTF-Ds 5 was able to estimate Ds more effectively for Latossolos Vermelhos (RMSE = 0.154 g cm^{-3}) (Table 5) and for land use systems, Forest formation (RMSE = 0.091 g cm-3) and Savanna formation (RMSE = 0.075 g cm-3) (Table 7). PTF-Ds 1 by Huf dos Reis et al. (2024) proved more effective in estimating Ds in soils with very clay texture with MMR of 0.206 g cm^{-3} and Pasture systems with MMR. of 0.160 g cm^{-3} (Table 6 and 7) and PTF-Ds 4 by Huf dos Reis et al. (2024) obtained lower MMR when estimating Ds for soils with Sandy clay loam texture (MSE = 0.148 g cm-3) (Table 6)

Table 5. Estimates of prediction uncertainties (Root Mean Square Error - RMSE) of soil density, by soil class of the soils studied in the basins of the Amambai, Iguatemi and Ivinhema Rivers in Mato Grosso do Sul.

Soil Class	Huf et al, 2024 - PTF-Ds 1	Huf et al, 2024 - PTF-Ds 2	Huf et al, 2024 - PTF-Ds 3	Huf et al, 2024 - PTF-Ds 4	Tomasella and Hodnett, 1998 - PTF-Ds 5	No of samples
			—RMSE—			
Argissolo Vermelho Amerelo	0.056	0.065	0.049	**0.043**	0.049	4.
Latossolo Vermelho	0.163	0.167	0.156	0.161	**0.154**	**75**
Neossolo Quartzarênico	0.121	0.140	0.084	0.102	**0.073**	4.
Plintossolo Argilúvico	0.291	0.277	0.313	**0.304**	0.307	5

Numbers in bold indicate the RMSEs for the most representative textural-class samples;
Source: authors.

Table 6. Estimates of prediction uncertainties (Root Mean Square Error - RMSE) of soil density, by textural class of the soils studied in the basins of the Amambai, Iguatemi and Ivinhema Rivers in Mato Grosso do Sul.

Textural Class	Huf et al, 2024 - PTF-Ds 1	Huf et al, 2024 - PTF-Ds 2	Huf et al, 2024 - PTF-Ds 3	Huf et al, 2024 - PTF-Ds 4	Tomasella and Hodnett, 1998 - PTF-Ds 5	No of samples
			—RMSE—			
Sand	0.118	0.133	**0.083**	0.095	0.067	3.
Loamy sand	0.099	0.105	0.081	0.080	**0.065**	8
Sandy clay	0.052	0.070	**0.036**	0.065	0.043	2.
Clay	0.219	**0.203**	0.229	0.209	0.261	5
Sandy clay loam	0.167	0.157	0.161	**0.148**	0.157	19
Sandy loam	0.409	0.396	0.401	**0.385**	0.397	16
Clay loam	**0.005**	0.098	0.045	0.170	0.115	1.
Very clay	**0.206**	0.216	0.207	0.219	0.212	34

Numbers in bold indicate the RMSEs for the most representative textural-class samples;
Source: authors.

Table 7. Estimates of prediction uncertainties (Root Mean Square Error - RMSE) of soil density, by land use of the soils studied in the basins of the Amambai, Iguatemi and Ivinhema Rivers in Mato Grosso do Sul.

Land Use	Huf et al, 2024 - PTF-Ds 1	Huf et al, 2024 - PTF-Ds 2	Huf et al, 2024 - PTF-Ds 3	Huf et al, 2024 - PTF-Ds 4	Tomasella and Hodnett, 1998 - PTF-Ds 5	No of samples
			—RMSE—			
Agriculture	0.313	0.339	**0.312**	0.337	0.339	10
Forest formation	0.120	0.118	0.111	0.109	**0.091**	35
Savanna formation	0.112	0.099	0.097	0.079	**0.075**	11
Mosaic of uses	0.172	0.148	0.169	0.151	**0.123**	5
Pasture	**0.160**	0.162	0.161	0.163	0.185	27

Numbers in bold indicate the RMSEs for the most representative textural-class samples;
Source: authors.

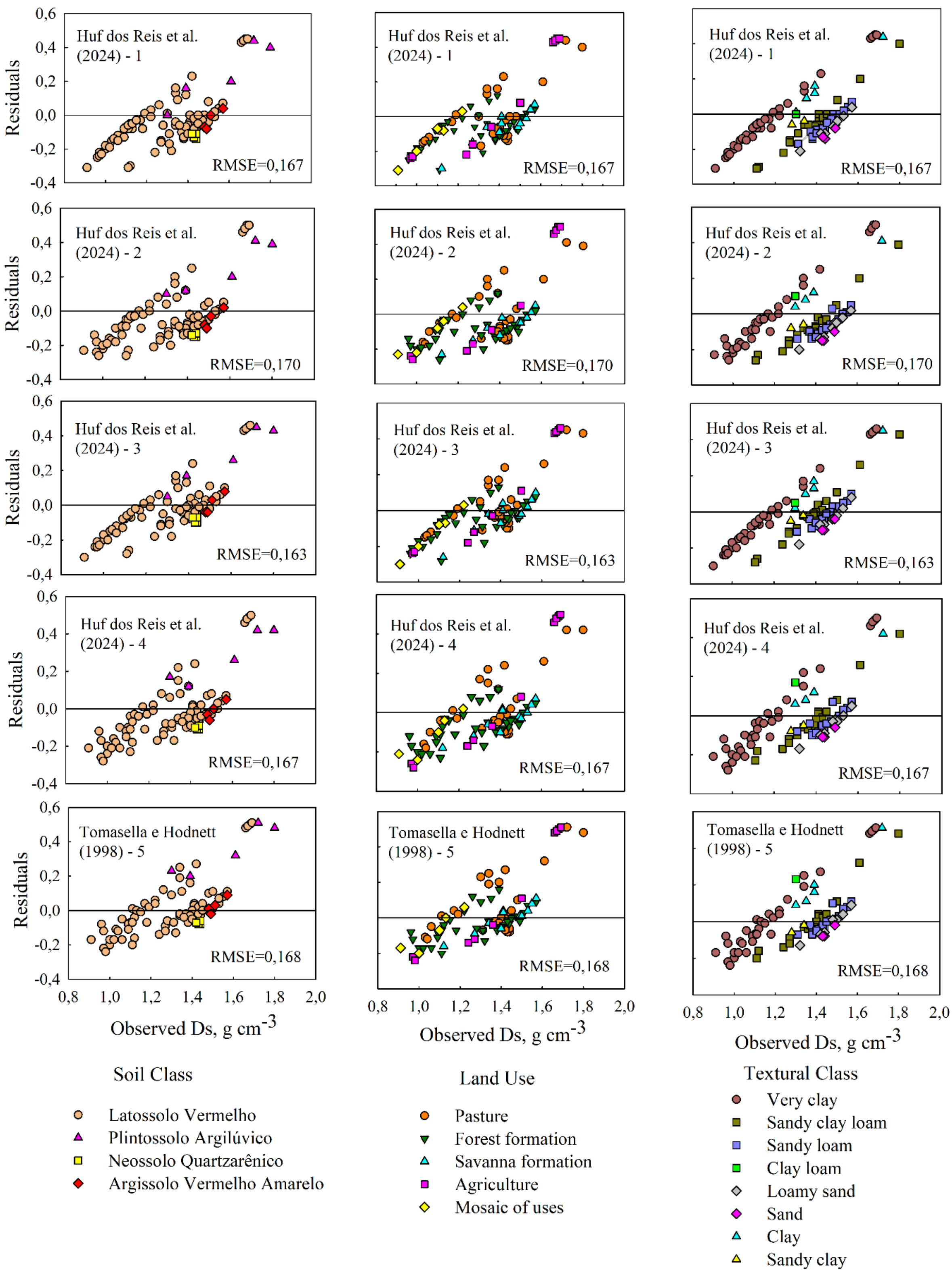

Figure 2. Dispersion of the residues *versus* density values observed by PTF-Ds 1, 2, 3 and 4 of Huf dos Reis et al. (2024) and PTF-Ds 5 of Tomasella and Hodnett (1998) of the soils studied in the basins of the Amambai, Iguatemi and Ivinhema Rivers in Mato Grosso do Sul, organized by textural class, soil class and land use.
Source: The authors.

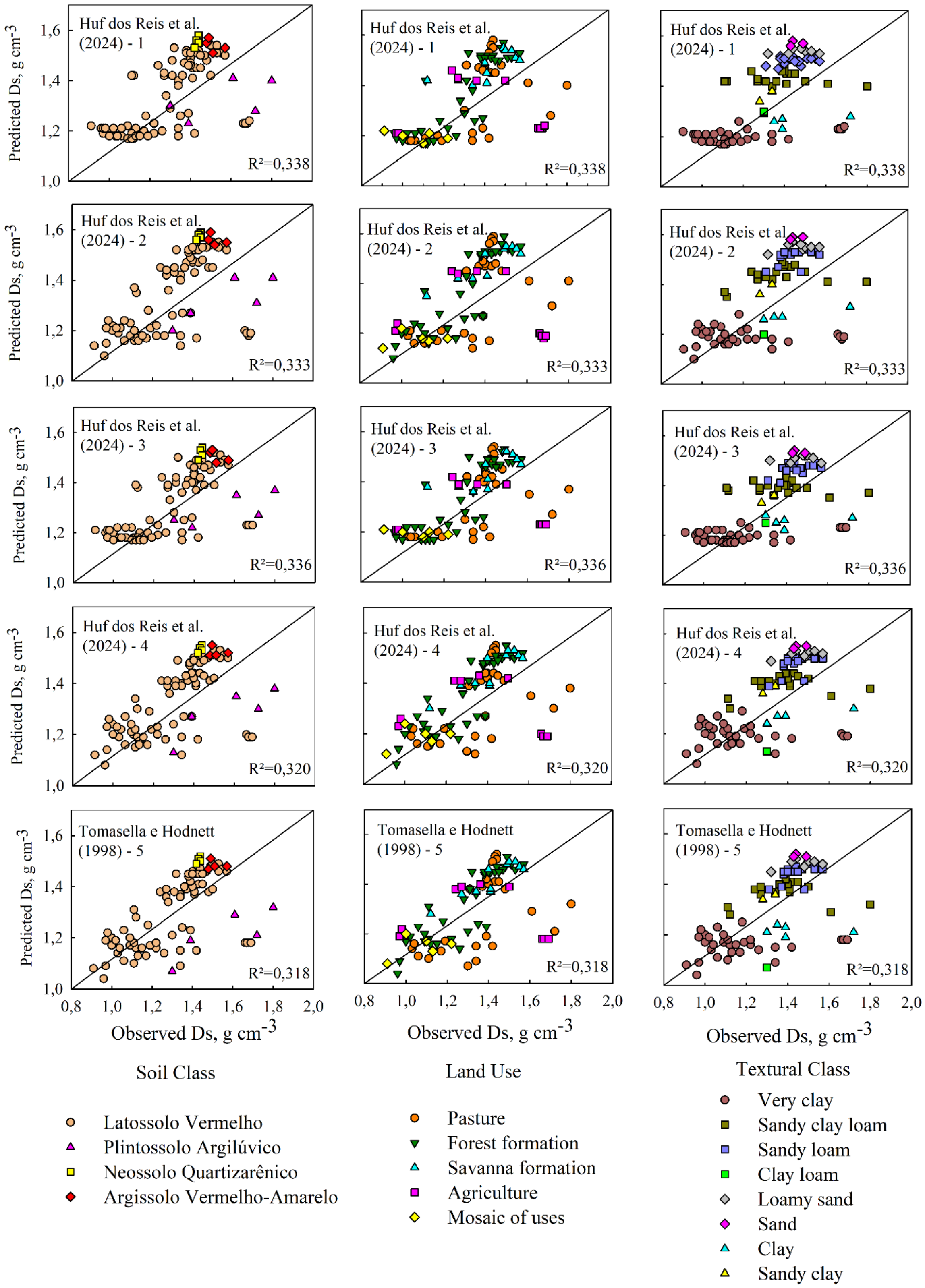

Figure 3. 1:1 dispersion graphs of the observed soil density values (Ds) *versus* Ds predicted by the PTF-Ds 1, 2, 3 and 4 of Huf dos Reis et al. (2024) and PTF-Ds 5 of Tomasella and Hodnett (1998) of the soils in the basins of the Amambai, Iguatemi and Ivinhema Rivers in Mato Grosso do Sul, classified by soil classes, textural classes and land use systems.
Source: The authors.

4 CONCLUSIONS

Among the eleven PTF-Ds assessed the most accurate were PTF-Ds 1, 2, 3 and 4 of Huf dos Reis et al. (2024) and PTF-Ds 5 of Tomasella and Hodnett (1998) with the smallest RMSE.

When estimating Ds for soils in Mato Grosso do Sul, PTF-Ds 3 by Huf dos Reis et al. (2024) is recommended when only particle size data are available. When the samples additionally given the organic carbon contents the PTF-Ds 4 from Huf dos Reis et al. (2024) tends to be the most accurate.

For estimation of Ds in soils of Mato Grosso do Sul with textural class Latossolo Vermelho, the PTF-Ds 5 of Tomasella and Hodnett (1998) tends to be the most accurate.

PTF-Ds 1 by Huf dos Reis et al. (2024) proved more accurate in soils with a very clay texture, and PTF-Ds 4 by Huf dos Reis et al. (2024) for soils with a Sandy clay loam texture.

It is recommended to adjust new PTFs-Ds for the area of the basins of the Amambai, Iguatemi and Ivinhema Rivers in the state of Mato Grosso do Sul, in particular with data from other soil classes besides the Latossolos Vermelhos, which consists of the largest percentage of data available for the region.

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