Soil Science/ Original Article

Pedotransfer functions for predicting soil-water retention under Brazilian Cerrado

Rafael de Andrade Carvalho Rosseti[1] (iD),
Ricardo Santos Silva Amorim[2] (iD),
Luis Augusto Di Loreto Di Raimo[3] (iD),
Gilmar Nunes Torres[4] (iD),
Lucas de Castro Moreira da Silva[2 ✉] (iD)
and Ianna Marília Alves[5] (iD)

[1] Empresa Mato-Grossense de Pesquisa, Assistência e Extensão Rural, Rua Cinquenta e Cinco, nº 454, Boa Esperança, CEP 78068-690 Cuiabá, MT, Brazil. E-mail: rafaelrosseti@empaer.mt.gov.br

[2] Universidade Federal de Viçosa, Departamento de Engenharia Agrícola, Campus Universitário, s/nº, Bela Vista, CEP 36570-000 Viçosa, MG, Brazil. E-mail: rsamorim@ufv.br, lucas.c.moreira@ufv.br

[3] Universidade Federal de Mato Grosso, Faculdade de Agronomia e Zootecnia, Programa de Pós-Graduação em Agricultura Tropical, Avenida Fernando Corrêa da Costa, nº 2.367, Boa Esperança, CEP 78060-900 Cuiabá, MT, Brazil. E-mail: luis.diloreto@hotmail.com

[4] Santos Lab Comércio e Indústria Aeroespacial Ltda., Avenida das Américas, nº 18.500, Sala 511, Recreio dos Bandeirantes, CEP 22790-704 Rio de Janeiro, RJ, Brazil. E-mail: gilmaragro@gmail.com

[5] Associação dos Produtores de Soja e Milho de Mato Grosso, Rua Engenheiro Edgar Prado Arze, nº 1.777, Centro Político Administrativo, CEP 78049-932 Cuiabá, MT, Brazil. E-mail: iannamarilia@hotmail.com

✉ Corresponding author

Abstract – The objective of this work was to determine pedotransfer functions to predict water retention at the -33 and -1500 kPa matric potentials of soils under Cerrado, in the south of the state of Mato Grosso, Brazil. Samples (n=156) were collected for model calibration (n=124) and validation (n=32). A stepwise multiple regression was used to determine pedotransfer functions. Willmott's index of agreement, root-mean-square error, Pearson's correlation coefficient, and the confidence index were used to evaluate the performance of the functions and to compare them with those described in the literature. The most efficient variables to estimate water retention were: microporosity, total sand, and clay at -33 kPa; and total sand, silt and clay at -1500 kPa. The regional pedotransfer functions explained more than 94% of water retention variance in the studied soils. The reliability of the functions to predict water retention increased, at -33 kPa, with the use of the structural property microporosity and, at -1500 kPa, with the use of granulometric parameters. The studied regional pedotransfer functions predict water retention at the -33 and -1500 kPa matric potentials of soils under Cerrado, in southern Mato Grosso, better than the functions described in the literature.

Index terms: available water capacity, field capacity, Oxisols, permanent wilting point, tropical soils.

Funções de pedotransferência para predição da retenção de água em solo sob Cerrado Brasileiro

Resumo – O objetivo deste trabalho foi determinar funções de pedotransferência para a predição da retenção de água nos potenciais matriciais -33 e -1500 kPa, em solos sob Cerrado, no sul do estado de Mato Grosso, Brasil. Amostras (n=156) foram coletadas para a calibração (n=124) e validação (n=32) dos modelos. Utilizou-se uma regressão múltipla passo a passo, para determinar as funções de pedotransferência. Utilizaram-se o índice de concordância de Willmott, a raiz do erro quadrático médio, o coeficiente de correlação de Pearson e o índice de confiança, para avaliar o desempenho das funções e compará-las com as descritas na literatura. As variáveis mais eficientes para estimar a retenção de água foram: microporosidade, areia total e argila a -33 kPa; e areia total, silte e argila a -1500 kPa. As funções de pedotransferência regionais explicaram mais de 94% da variância da retenção de água nos solos estudados. A confiabilidade da predição da retenção de água, -33 kPa, aumentou com o uso da propriedade estrutural microporosidade e, a -1500 kPa, com o uso de parâmetros granulométricos. Funções de pedotransferência regionais predizem melhor a retenção de água nos potenciais matriciais -33 e -1500 kPa, em solos sob Cerrado, no sul de Mato Grosso, do que as funções descritas na literatura.

Termos para indexação: capacidade de água disponível, capacidade de campo, Latossolos, ponto de murcha permanente, solos tropicais.

Introduction

Plant available water capacity (PAWC) is described as the soil capacity to retain water and make it available for roots uptake. Some recognized practical uses for PAWC are land-use planning, such as irrigation projects, agricultural zoning, water balance, and others (Silva et al., 2014). PAWC is defined as the soil moisture (θ) between an upper limit and a lower limit, represented by the soil-water content at field capacity and permanent wilting point, respectively.

Knowing PAWC is essential for the assessment of soil available water and soil-water storage, and it is an important information for efficient management of agricultural crops (Silva et al., 2014; Qiao et al., 2019). Nevertheless, determining the soil-water retention properties through conventional methods can be time-consuming and costly (Botula et al., 2014; Santra et al., 2018), besides being unfeasible for soil and crop management. To overcome this limitation, in the last decades, alternative methods have been sought to measure these complex soil properties (Botula et al., 2014), such as pedotransfer functions (pedofunctions).

Pedofunctions are an alternative method to estimate complex soil attributes, such as water retention properties, from easily and/or inexpensively measured properties. Pedofunctions are considered a feasible approach for determining soil-water retention properties (Rab et al., 2011); however, a greater reliability for their specific use is still necessary, to reduce the prediction errors, specific pedofunctions should not be extrapolated beyond the soil classes for which they were determined, since the more homogeneous is the pedofunction database, the better is the model performance, according to Souza et al. (2014).

Applying pedofunctions in different edaphic conditions from which they were determined can cause loss of accuracy, due to soil property particularities in each region (Minasny et al., 1999). Thus, considering the specificities of Brazilian soils, such as structure and mineralogy, especially in the Cerrado biome (Severiano et al., 2013; Martinez & Souza, 2020), some studies have been carried out to generate and validate pedofunctions for soil-water retention in Brazil (Botula et al., 2014; Ottoni et al., 2018). An important information on pedotransfer functions used for Brazilian soils is summarized in a study highlighting the particularities of highly weathered tropical soils, suggesting a judicious use of pedofunctions by Ottoni et al. (2018). These authors emphasized the ineffectiveness of pedofunctions made for temperate soils in predicting Brazilian soil properties, and they recommend the use of specific pedofunctions determined through a Brazilian soil database to predict Brazilian soils attributes.

Although many efforts have been made to upgrade the prediction for water retention of Brazilian soils, such as the establishment of the Hydrophysical Database for Brazilian Soils (Hybras) (Ottoni et al., 2018), improvements are still needed. For instance, the Hybras library does not contain data from the state of Mato Grosso, which is responsible for 26.3% of the Brazilian grain harvest and still has great potential for expanding production (Imea, 2015). Therefore, it is necessary to fit pedofunctions to estimate soil-water retention for Cerrado soils of southern Mato Grosso. Considering that regional-specific pedofunctions can be more accurate in the prediction of soil-water retention for the southern region of Mato Grosso than the current pedofunctions available in the literature.

The objective of this work was to determine pedotransfer functions to predict water retention at the -33 and -1500 kPa matric potentials of soils under Cerrado, in the south of the state of Mato Grosso, Brazil.

Materials and Methods

The study was developed in the southern region of the state of Mato Grosso. Within the Mid-West region of Brazil, Mato Grosso state covers an area of approximately 93 million hectares (IBGE, 2015). Mato Grosso state has a characteristic hot and semi-humid tropical climate, with average temperature between 18 and 24°C, whose annual maximum is 34°C, with wet summers and dry winters (May to September). The annual precipitation ranges from 1,200 to 2,000 mm, and the highest values are observed in the north and mid-north regions of the state and in regions at altitudes close to 800 m. The main soil classes (79%) in Mato Grosso state are Latossolos, Argissolos, and Neossolos, according to Santos et al. (2013), which corresponds to Oxisols, Ultisols, and Entisols, respectively, by the USDA Soil Taxonomy (Soil Survey Staff, 2014), covering respectively 41%, 25%, and 13% of the state surface (Di Raimo et al., 2019).

A data set of 156 disturbed and undisturbed soil samples was used. For the field survey carried out in the central-south region of the state of Mato Grosso, soil samples were collected at 0–10, 10–20, 20–30, 20–40, 35–45, and 40–60 cm soil depths, covering the four main soil classes in the region, which are Argissolos, Cambissolos, and Gleissolos (Oxisols, Ultisols, Entisols, and Inceptisols, respectively). The undisturbed samples were collected with the aid of volumetric cylinders and a Kopeck sampler for the determination of the following soil properties: macroporosity (Mac), microporosity (Mic), bulk density (Bd), and soil moisture at -33 kPa (θ_{33}) matric potential. Disturbed samples were collected with a Dutch auger for the determination of soil texture, particle density (Pd), total organic carbon content (TOC), and soil moisture at -1500 kPa (θ_{1500}) matric potential. Laboratory procedures were carried out according to the method described by Teixeira et al. (2017). For the soil texture analysis, the pipette method was used, Pd was obtained by the volumetric flask method, and Bd was obtained by the core method. Total porosity (Tp) was calculated from the following equation: [1 - (Bd/Pd)].

Soil Mic was determined by saturating and subjecting the undisturbed soil samples to 6 kPa matric potential, and Mac was calculated by the difference between Tp and Mic. The undisturbed samples were subjected to the Richards extractor (Klute, 1986) at -33 kPa potential. Gravimetric moisture for the -1500 kPa matric potentials was determined by the WP4 psychrometer (Gubiani et al., 2014), using disturbed samples. Gravimetric moisture was multiplied by Bd, to obtain the volumetric moisture of each sampled soil layer. Total organic carbon (TOC) was quantified by the wet oxidation of organic matter, using a solution of potassium dichromate in an acid medium, with an external source of heat.

Dataset values (mean, minimum, maximum, and standard deviation) are presented for each soil class (Table 1). The dataset used for pedofunction calibration and validation includes the following textural classes of the 156 soil samples: very clayey, clay, sandy clay loam, silty loam, sandy loam, loamy sand, and sand are shown in the textural triangle (Figure 1).

To obtain location-specific information, the pedofunctions were determined in two steps: fitting pedofunctions that are named "Rosseti", from the study

Table 1. Descriptive statistics for soil properties database, separated by soil class.

Soil class		Bd (g cm⁻³)	Total sand (g kg⁻¹)	Silt (g kg⁻¹)	Clay (g kg⁻¹)	Tp (cm³ cm⁻³)	Mac (cm³ cm⁻³)	Mic (cm³ cm⁻³)	TOC (%)	θ_{33} (cm³ cm⁻³)	θ_{1500} (cm³ cm⁻³)
Ultisol	MD	1.12	201.3	351.1	447.7	0.54	0.19	0.35	1.87	0.31	0.22
	SD	0.14	44.3	61.9	104.2	0.07	0.07	0.04	0.89	0.05	0.04
	MN	1.03	169.9	310.3	292.8	0.44	0.12	0.31	1.18	0.26	0.16
	MX	1.33	265.1	442.0	519.8	0.59	0.28	0.39	2.87	0.38	0.26
Inceptisol	MD	1.48	771.6	60.4	167.9	0.40	0.13	0.26	1.43	0.19	0.09
	SD	0.04	12.7	3.5	11.0	0.02	0.03	0.04	0.78	0.02	0.00
	MN	1.46	759.6	56.9	158.2	0.39	0.10	0.24	0.65	0.17	0.09
	MX	1.52	785.0	63.8	179.8	0.42	0.15	0.31	3.65	0.21	0.10
Red-yellow Oxisol	MD	1.18	275.3	187.9	536.8	0.57	0.14	0.43	2.08	0.36	0.16
	SD	0.15	178.1	76.0	133.0	0.06	0.05	0.07	1.14	0.07	0.04
	MN	0.81	142.7	23.2	159.8	0.36	0.04	0.16	0.64	0.09	0.04
	MX	1.57	917.0	340.5	744.5	0.74	0.25	0.54	7.94	0.45	0.26
Red Oxisol	MD	1.19	236.0	253.5	510.5	0.51	0.13	0.38	1.11	0.32	0.23
	SD	0.03	39.9	70.7	110.2	0.02	0.04	0.02	0.75	0.02	0.01
	MN	1.15	200.2	200.6	387.2	0.49	0.09	0.35	0.51	0.30	0.22
	MX	1.22	279.0	333.8	599.2	0.52	0.17	0.40	1.95	0.34	0.25
Entisol	MD	1.52	880.9	17.2	101.9	0.45	0.30	0.15	0.67	0.11	0.03
	SD	0.09	23.5	10.5	19.8	0.04	0.04	0.04	0.36	0.04	0.01
	MN	1.28	791.6	0.2	28.2	0.35	0.16	0.08	0.25	0.06	0.01
	MX	1.67	960.4	46.8	115.4	0.53	0.38	0.30	1.84	0.26	0.08

[1]Bd, bulk density; Tp, total porosity; Mac, macroporosity; Mic microporosity; TOC, total organic carbon; θ_{33}, moisture at -33 kPa matric potential; θ_{1500}, moisture at -1500 kPa matric potential; MD, mean; SD, standard deviation; MN, minimum; MX, maximum.

database; and performance evaluation and comparison with pedofunctions generated in other regions, available in the literature. The stepwise multiple linear regression method was used to fit the pedofunctions. Only independent variables that significantly (p<0.05) contribute to a dependent variable description were included in the models. Out of total dataset, 80% was used for calibration step (n=124), and 20% (n=32) for validation (Figure 1).

The independent variables in the regression models were: Ds, AT, Silt, Clay, Tp, Mic, Mac, and TOC. The residual moisture at -33 and -1500 kPa matric potentials were inserted as dependent variables. Notably, the potentials -6, -10, and -33 kPa have been used arbitrarily, to estimate field capacity (Ottoni Filho et al., 2014); however, based on recent findings from studies assessing Brazilian soils, the potentials -6 kPa and -10 kPa are commonly used (Andrade & Stone, 2011; Silva et al., 2014; van Lier & Wendroth, 2016; Turek et al., 2020). The soil moisture was predicted at -33 kPa, which is the "classical" matric potential, as used in a national scope by Ottoni et al. (2018). The potential of -33 kPa for field capacity determination stands out for being more conservative, which may influence its practical use (Silva et al., 2014).

The pedofunctions from other studies used for comparison were chosen considering the soil attributes available in the present study database (Table 2). For the
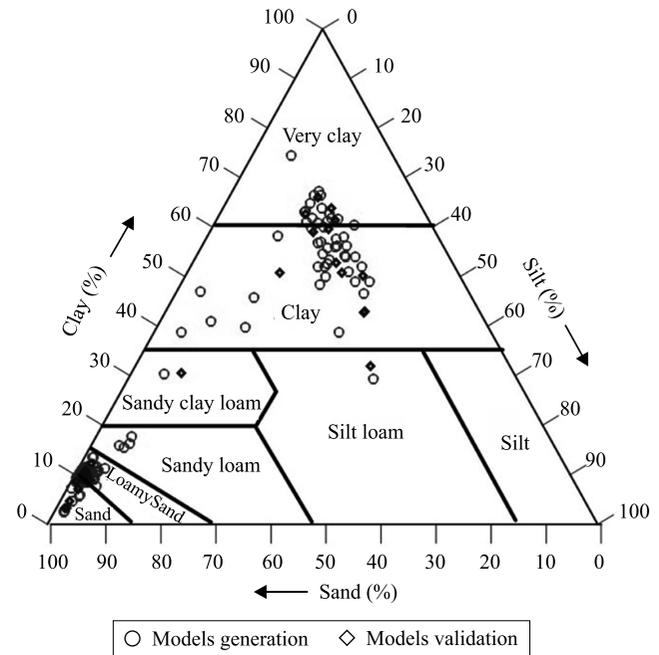

Figure 1. Textural classes of soil samples used to generate and validate the Rosseti pedotransfer functions. N = 156.

Table 2. Pedofunctions described in the literature and the obtained pedofunctions (Rosseti) to estimate the soil moisture at -33 kPa (θ_{33}) and 1500 kPa (θ_{1500}) matric potentials.

Source	Equation	R²
Lal (1978)	$\theta_{33} = 0.334 - 0.003$ TS	0.65
	$\theta_{1500} = 0.247 - 0.003$ TS	0.69
Giarola et al. (2002)	$\theta_{1500} = -0.031 + 0.005$ Silt $+ 0.003$ Clay	0.81
Urach (2007)	$\theta_{33} = 0.643 - 0.000238$ TS $- 0.26767$ Bd	0.68
	$\theta_{1500} = 0.462 - 0.00022$ TS $- 0.000074$ Silt $- 0.1838$ Bd	0.77
Nascimento et al. (2010)	$\theta_{33} = 0.0409 + 0.000377$ Clay $+ 0.000108$ Silt	0.69
	$\theta_{1500} = 0.0221 + 0.000288$ Clay	0.76
Souza et al. (2014) Tilled soil	$\theta_{33} = 0.15839 + 0.00031$ Clay $- 0.00240$ Mic	0.86
	$\theta_{1500} = 0.13636 + 0.00028$ Clay $- 0.00244$ Mic	0.89
Souza et al. (2014) Not tilled soil	$\theta_{33} = 0.08595 + 0.006102$ Mac	0.61
	$\theta_{1500} = 0.0591 + 0.00646$ Mac	0.59
Rosseti 1	$\theta_{33} = 0.264 - 0.002$ TS $+ 0.024$ TOC $+ 0.002$ Clay	0.94
	$\theta_{1500} = 0.386 - 0.004$ TS $- 0.002$ Clay	0.94
Rosseti 2	$\theta_{33} = 0.057 - 0.001$ TS $+ 0.743$ Mic	0.98
	$\theta_{1500} = 0.568 - 0.003$ TS $- 0.001$ Clay $- 0.281$ Tp $- 0.069$ Bd $+ 0.005$ TOC	0.95

R², coefficient of determination; TS, total sand (%); Silt (%); Clay (%); Bd, bulk density (g cm⁻³); Tp, total porosity (cm³ cm⁻³); Mac, macroporosity (cm³ cm⁻³); Mic, microporosity (cm³ cm⁻³); θ_{33}, soil moisture at -33 kPa (cm³ cm⁻³); θ_{1500}, soil moisture at -1500 kPa (cm³ cm⁻³).

validation process, the following statistical parameters were used: the Willmott's agreement index (d), root-mean-square error (RMSE), and the confidence index (c), in the equations (1), (2) and (3) respectively:

$$d = 1 - \left[\sum_{i=1}^{n} (E_i - O_i)^2 \right] \Big/ \left[\sum_{i=1}^{n} \left(|E_i - \overline{O}| + |O_i - \overline{O}| \right)^2 \right] \quad (1)$$

$$RMSE = \left[\sum_{i=1}^{n} (O_i - E_i)^2 / n \right]^{0.5} \quad (2)$$

$$c = r \times d \quad (3)$$

in which: d is the Willmott's agreement index; E_i is the estimated value; O_i is the observed value; RMSE is the root-mean-square error; n is the total number of observed and estimated value pairs; c is the confidence index; and r is the Pearson's correlation coefficient.

Results and Discussion

Soil attributes had very significant correlation coefficients for both θ_{1500} and θ_{33} estimates (Table 3). The highest correlation coefficients for θ_{33} occurred between total sand, clay, and microporosity, and, for θ_{1500}, between total sand, silt, and clay. These results show the significant influence of soil granulometric composition on soil-water retention in both observed potentials, which is also noted by Urach (2007) and Souza et al. (2014), in different environmental conditions. However, there is a high correlation and, consequently, high importance of soil structural variables (total porosity, microporosity, and macroporosity) to predict θ_{33}.

The pedofunction Rosseti 2 fitted for θ_{1500} with the variables total sand, clay, total porosity, bulk density, and total organic carbon, while the variables used for fitting θ_{33} were microporosity and total sand. By these results, it can be stated that the inclusion

of microporosity in the Rosseti 2 improved the θ_{33} estimation with a higher R^2 (0.982) than that of Rosseti 1 (0.939). However, including structural attributes did not bring great benefits from using Rosseti 2 instead of Rosseti 1 for θ_{1500}, as there was a slight increase of R^2 from 0.942 to 0.952. This result does not justify the labor demand for gathering more complex data (for instance, structural variables), when the goal is to estimate θ_{1500}.

Overall, Rosseti 1 and 2 performed better than the generic models available in the literature for predicting θ_{33} and θ_{1500} of a Cerrado soil database (Figure 1 and 3). The models from literature that predict water retention of Cerrado soils, with a closer performance to the specific Rosseti pedofunctions were obtained by Lal (1978) for θ_{33}, with RMSE=0.09 and d=0.87, and for θ_{1500}, in the models proposed by Lal (1978), with RMSE=0.04 and d=0.95, and in the models determined by Giarola et al. (2002), with RMSE=0.05 and d=0.93, which is in agreement with the present study. Minasny et al. (1999), Nascimento et al. (2010), Souza et al. (2014), and Ottoni et al. (2018) reported that pedofunctions perform better when determined and applied for specific regions, instead of applying them in different conditions from which they were generated.

The models that used the equations proposed by Souza et al. (2014) and Nascimento et al. (2010) had the greatest errors in the prediction of water retention of Cerrado soils. This result is explained by the difference of environments where the studies were developed, since both studies used a soil database from the Brazilian coastal tablelands while the present study was developed for soils under the Cerrado biome. These two environments have several distinctions in a wide range of variables, especially the pedological ones. Soils from the coastal tablelands

Table 3. Pearson's correlation coefficients (r) and significance between dependent variables (soil moisture at -33 kPa and -1500 kPa matric potentials of) and independent variables.

Matric potential		Bd (g cm⁻³)	Total sand (%)	Silt (%)	Clay (%)	Tp (cm³cm⁻³)	Mac (cm³cm⁻³)	Mic (cm³cm⁻³)	TOC (%)
θ_{33}	r	-0.88**	-0.96**	0.84**	0.95**	0.84**	-0.87**	0.99**	0.75**
	N	124	124	124	124	124	124	124	120
θ_{1500}	r	-0.88**	-0.96**	0.92**	0.93**	0.76**	-0.79**	0.90**	0.65**
	N	124	124	124	124	124	124	124	120

Bd, bulk density; Tp, total porosity; Mac, macroporosity; Mic, microporosity; TOC, total organic carbon; θ_{33}, soil moisture at 33 kPa (cm³ cm⁻³); θ_{1500}, soil moisture at 1500 kPa (cm³ cm⁻³). N, sample size. **Significant at 1% probability.

are, in general, known for their cohesive character in subsurface horizons (Gomes et al., 2017), which implies several peculiarities in their physical behavior, such as poor drainage and low soil porosity in the cohesive horizons (Gomes et al., 2012; Mota et al., 2018). When considering the Cerrado soils, especially Oxisols (Latossolos), which is the predominant soil class, high macroporosity and high permeability were observed, even in soils with very clayey texture (Silva et al., 2015, 2019).

Despite the great distinction between soils from the different Brazilian geoenvironmental units, the equations proposed by Giarola et al. (2002) and Urach et al. (2007), developed in southern Brazil, had a lower error for predicting water retention of the Cerrado soils than the studies carried out by Nascimento et al. (2010) and Souza et al. (2014). The results are explained by the database used in Giarola et al. (2002) and Urach et al. (2007), which covered several soil classes, while Nascimento et al. (2010) and Souza et al. (2014) used specific soil databases from the Brazilian coastal tablelands, as already mentioned.

The model proposed by Lal (1978), despite being formulated in another country, showed less error in the prediction of water retention for the soils in the Cerrado of Mato Grosso than the models determined for the coastal tablelands. Although Lal's (1978) study was carried out in Nigeria, the soil database had
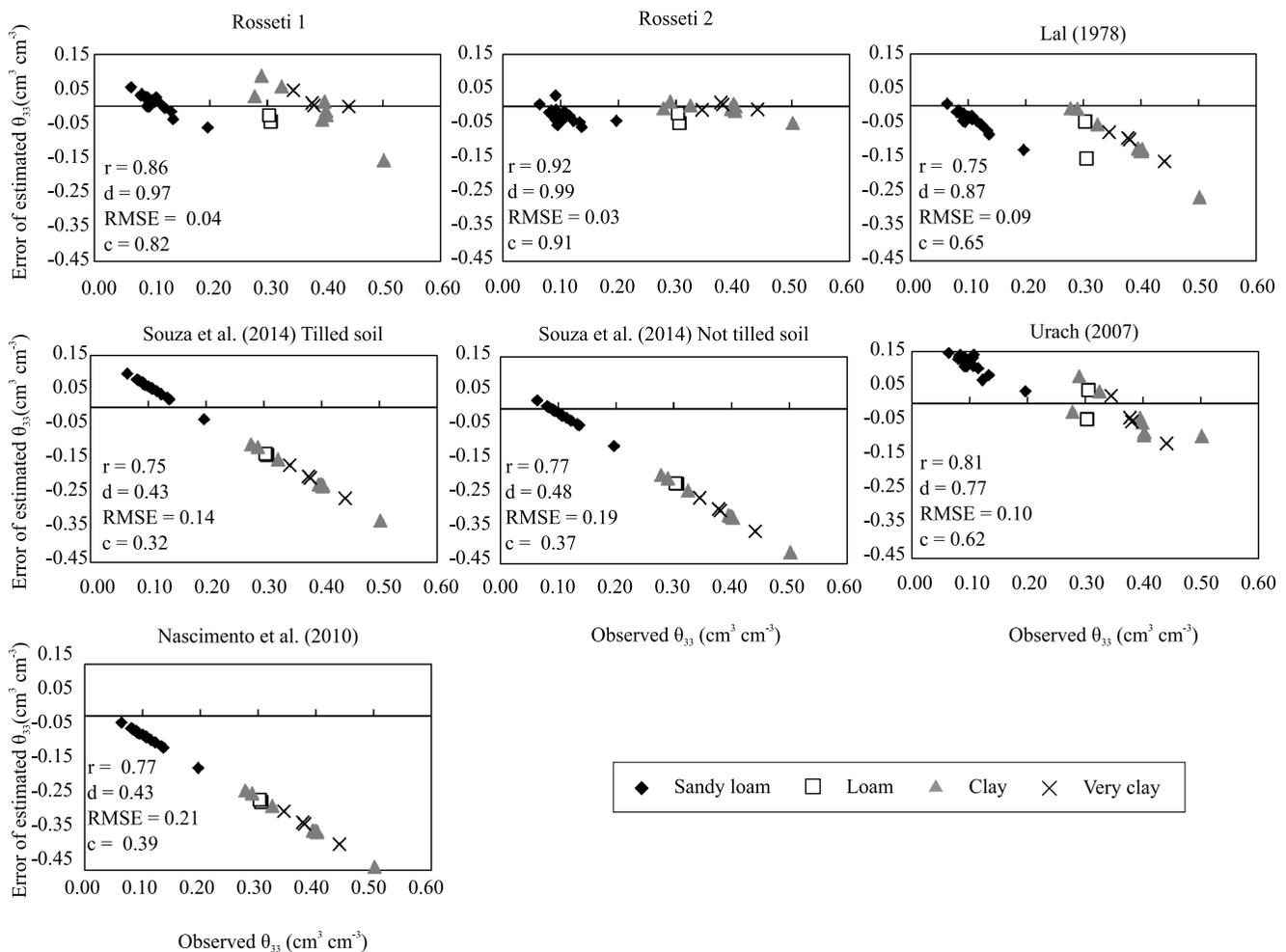

Figure 2. Estimated errors for the prediction of pedotransfer functions of moisture at -33 kPa (θ33) matric potential and model performance indexes [correlation coefficient (r), the Willmott's agreement index (d), root-mean-square error (RMSE), and confidence index (c)].

similar clay mineralogy, composed mainly by kaolinite and sesquioxides, like Cerrado soils mineralogy, especially concerning Oxisols (Martinez & Souza, 2020). Nevertheless, the Rosseti models were proved to have the best accuracy.

The best fit of the Rosseti pedofunctions reinforces the demand to determine location-specific equations for accurate prediction of soil attributes, at least while generic pedofunctions are not formulated and validated in representative databases, as highlighted by Patil & Singh (2016). The results of the present study contribute to studies with similar goals developed in the Cerrado biome, such as those by Andrade & Stone (2011) and Medrado & Lima (2014), and they can be compared with other functions determined in

the region, to establish a generic and representative regional function of the Brazilian Cerrado.

The regional pedofunctions determined in the present study can explain more than 94% of the θ_{33} and θ_{1500} variance; therefore, the models satisfactorily predict water retention at 33 and 1500 kPa matric potentials of. It is noteworthy that the θ_{33} prediction should be made based on equations that use structural soil parameters (for instance, soil porosity) as input data, since these variables can be more easily modified according to land use. However, for θ_{1500} estimates, equations that input only soil texture parameters can be used, since θ_{1500} is under the influence of soil textural porosity, which is little modified with land use and management.
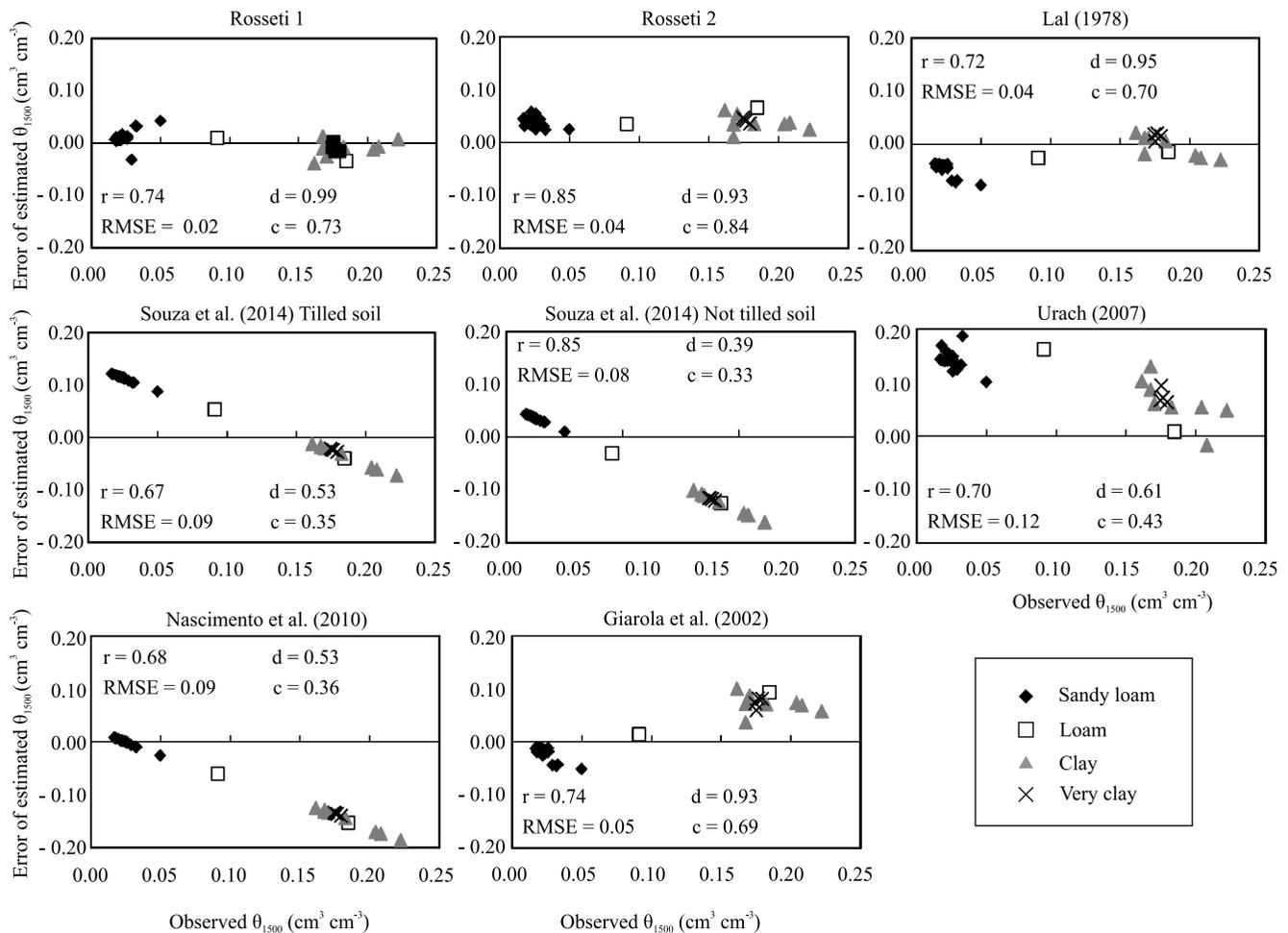

Figure 3. Estimated errors for the prediction of pedotransfer functions of moisture at -1500 kPa (θ_{1500}) matric potential and model performance indexes [(the correlation coefficient (r), the Willmott's agreement index (d), root-mean-square error (RMSE), and confidence index (c)].

Conclusions

1. Regional pedotransfer functions for soils under Cerrado, in southern Mato Grosso state, predict water retention at -33 and -1500 kPa better than functions described in the literature.

2. The use of soil structural properties improves the prediction of water retention at -33 kPa, but it does not show accuracy gain for water retention at -1500 kPa.

3. The best equation to predict the moisture at -33 kPa for Cerrado soils of southern Mato Grosso is: $\theta_{33} = 0.057 - 0.001 \times$ total sand $+ 0.743 \times$ microporosty.

4. The best and more parsimonious equation to predict water retention at -1500 kPa for Cerrado soil of southern Mato Grosso is: $\theta_{1500} = 0.386 - 0.004 \times$ total sand $- 0.002 \times$ clay.

Acknowledgments

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