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## Pedotransfer functions of soil water properties to estimate the S-index

João H. Caviglione<sup>1</sup>

<sup>1</sup> Instituto Agrônômico do Paraná/Área de Solos. Londrina, PR. E-mail: [caviglione@iapar.br](mailto:caviglione@iapar.br) (Corresponding author) - ORCID: 0000-0002-2518-0031

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soil-water retention curve  
Akaike information criterion  
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van Genuchten-Mualem

### ABSTRACT

One big challenge for soil science is to translate existing data into data that is needed. Pedotransfer functions have been proposed for this purpose and they can be point or parametric when estimating the water retention characteristics. Many indicators of soil physical quality have been proposed, including the S-Index proposed by Dexter. The objective of this study was to assess the use of pedotransfer functions for soil water retention to estimate the S-index under field conditions in the diversity of soils of the Paraná state. Soil samples were collected from 36 sites with textures ranging from sandy to heavy clay in the layers of 0-0.10 and 0.10-0.20 m and under two conditions (native forest and cultivated soil). Water content at six matric potentials, bulk density and contents of clay, sand and silt were determined. Soil-water retention curve was fitted by the van Genuchten-Mualem model and the S-index was calculated. S-index was estimated from water retention curves obtained by the pedotransfer function of Tomasella (point and parametric). Although the coefficient of determination varied from 0.759 to 0.895, modeling efficiency was negative and the regression coefficient between observed and predicted data was different from 1 in all comparisons. Under field conditions in the soil diversity of the Paraná state, restrictions were found in S-index estimation using the evaluated pedotransfer functions.

### Palavras-chave:

curva de retenção de água do solo  
critério de informação de Akaike  
estrutura do solo  
van Genuchten-Mualem

## Funções de pedotransferência de propriedades hídricas do solo para estimar o Índice S

### RESUMO

Um grande desafio na ciência do solo é traduzir os dados existentes em dados que se necessita. Para tanto, foram propostas as funções de pedotransferência, que podem ser pontuais ou paramétricas quando estimam as características de retenção de água. Vários indicadores foram propostos para a qualidade física de solo; entre eles, o índice S proposto por Dexter. O objetivo deste estudo foi avaliar a utilização de funções de pedotransferência para retenção de água no solo para estimar o índice S em condições de campo na diversidade de solos do Paraná. Amostras de solos foram coletadas de 36 locais com as texturas variando de arenosa a muito argilosa, nas camadas de 0 a 0,10 e 0,10 a 0,20 m e em duas condições (mata nativa e solo explorado). Determinaram-se o conteúdo d'água em seis potenciais mátricos, densidade do solo, teores de argila, de areia e de silte. A curva de retenção de água foi ajustada pelo modelo van Genuchten-Mualem e o índice S calculado. O índice S foi estimado das curvas de retenção de água obtidas pela função de pedotransferência de Tomasella (pontual e paramétrica). Embora o coeficiente de determinação tenha variado entre 0,759 a 0,895, o índice de eficiência da modelagem foi negativo e o coeficiente de regressão entre observado e predito foi diferente de 1 em todas as comparações. Nas condições de campo e diversidade de solos do Paraná, foram encontradas restrições na estimativa do índice S usando as funções de pedotransferência avaliadas.



## INTRODUCTION

Bouma (1989) introduced the term Pedotransfer Functions (PTFs) to define predictive functions of soil attributes of expensive or difficult determination, which are obtained using available data and also considering existing information from soil surveys. Nevertheless, PTFs began to be used also with topographic and spatial data (Motaghian & Mohammadi, 2011).

PTFs to determine hydraulic conductivity and soil-water retention curve (SWRC) are the most common ones, and PTFs have also been developed for resistance to penetration (Almeida et al., 2012), bulk density (Hollis et al., 2012), electrical resistivity (Hadzick et al., 2011) and erodibility in soil loss model (Silva et al., 2016).

Nguyen et al. (2017) described 3 groups of PTFs for SWRC. The first group (point-PTFs) estimates soil moisture at specific matric potentials. The second group (parametric PTFs) determines SWRC parameters and, in this group, the van Genuchten-Mualem (VGM) model is probably the most widely used model according to Vereecken et al. (2010). The third group (physical-conceptual PTFs), little used due to the limitations, predicts hydraulic properties based on a structural model of the soil.

S-index is described as the tangent (slope) of the SWRC at its inflection point and was proposed by Dexter (2004) as an indicator of soil physical quality. Andrade & Stone (2009) proposed the value of 0.045 as the limit of good structural quality of Cerrado soils. However, the process of determining soil moisture and obtaining SWRC by Richards' pressure plate apparatus is normally time-consuming, especially at the highest tensions, when it may last months.

This study aimed to verify the viability of using pedotransfer functions of SWRC to estimate S-index under field conditions in the diversity of several soils of the Paraná state.

## MATERIAL AND METHODS

Soil samples were collected in 36 sites in the Paraná state, in two layers (0-0.10 and 0.10-0.20 m) under the conditions of native forest and cultivated soil. Management and crop of each site are representative of the region and the sites are close to one another, totaling 144 conditions. Management was defined by the owner of each site.

No-tillage occurred in 12 sites, conventional planting in 21 sites and pasture in 3 sites. In sites under no-tillage, the crops were soybean (6 sites) and corn (6 sites). In sites under conventional planting, the crops were corn (14 sites), soybean (3 sites), sorghum (1 site), royal palm (1 site), cassava (1 site) and peach palm (1 site).

The sampled sites were located in the municipalities of: Apucarana, Bandeirantes, Bela Vista do Paraíso, Cambará, Campo Mourão, Cândido de Abreu, Cascavel, Cerro Azul, Cianorte, Diamante do Norte, Francisco Beltrão, Guaíra, Guarapuava, Guaraqueçaba, Iporã, Irati, Jaguaçu, Joaquim Távora, Lapa, Laranjeiras do Sul, Londrina, Mauá da Serra, Morretes, Nova Cantu, Palmas, Palotina, Paranavai, Pato Branco, Planalto, Ponta Grossa, Quedas do Iguaçu, Santa

Helena, São José dos Pinhais, São Miguel do Iguaçu, Telêmaco Borba and Umuarama, all in the Paraná state, with the delimitation of the morpho-physiographic regions (Figure 1).

For each condition (management, site and layer), undisturbed samples were collected in triplicate, within a distance that ensured sampling representativeness. Steel rings (99.37 cm<sup>3</sup>) were vertically inserted into the soil using a manual device specifically built for this purpose. A total of 432 subsamples were collected, and samples were also collected for physical analysis.

Bulk density (Ds) and gravimetric moisture content at tensions (matric potentials) of 6, 30, 100, 300, 500 and 1,500 kPa, on tension table or Richards' pressure-plate apparatus, were determined to fit the soil-water retention curve. Clay, sand and silt contents (Table 1) were determined by the pipette method with slow agitation (Donagema et al., 2011).

The SWRC was fitted by the VGM model, described in Eq. 1 (Genuchten, 1980), maintaining the Mualem restriction.

$$\theta_h = (\theta_{sat} - \theta_{res}) \left[ 1 + (\alpha h)^n \right]^{-m} + \theta_{res} \quad (1)$$

where:

- $\theta_h$  - soil moisture content at tension  $h$ , g g<sup>-1</sup>;
- $\theta_{sat}$  - saturated soil moisture content, g g<sup>-1</sup>;
- $\theta_{res}$  - residual soil moisture content, g g<sup>-1</sup>; and,
- $m$ ,  $n$  and  $\alpha$  - parameters.

S-index is described as the tangent (slope) of the SWRC at its inflection point. When the VGM model is adopted with the Mualem restriction ( $m = 1 - 1/n$ ), S-index can be obtained by Eq. 2, in absolute value, with the parameters of Eq. 1 (Dexter, 2004).

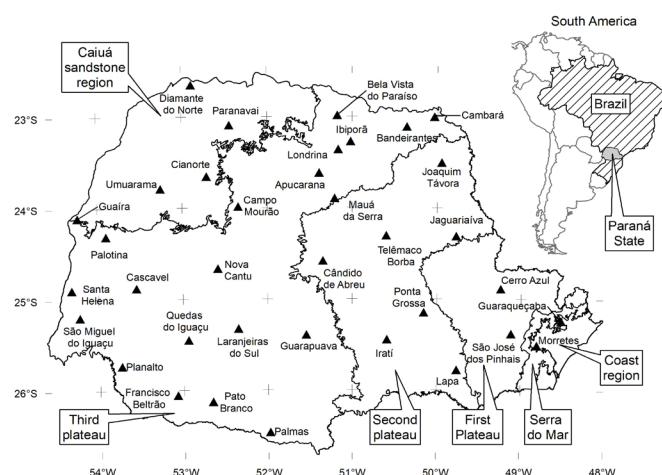


Figure 1. Distribution of the sampled sites and morpho-physiographic regions in the Paraná state

Table 1. Descriptive statistics of physical analyses of the 144 conditions

Attribute	Mean	Standard deviation	Median	Maximum	Minimum
Clay <sup>1</sup>	498.0	232.0	570.0	810.0	50.0
Silt <sup>1</sup>	148.0	84.0	150.0	430.0	10.0
Sand <sup>1</sup>	354.0	267.0	280.0	930.0	70.0
Density <sup>2</sup>	1.15	0.21	1.12	1.69	0.91

<sup>1</sup>Clay, silt and sand contents, g kg<sup>-1</sup>; <sup>2</sup>Soil bulk density, kg dm<sup>-3</sup>

$$S = -n(\theta_{\text{sat}} - \theta_{\text{res}}) \left( \frac{2n-1}{n-1} \right)^{\left( \frac{1}{n-2} \right)} \quad (2)$$

where:

S - S-index proposed by Dexter (2004).

SWRCs were fitted with field-observed data and data estimated by the PTFs of Tomasella et al. (2003), who developed point and parametric PTFs based on Brazilian soils. Point PTF estimates 6 points of tension, at 0 (saturation), 6, 10, 33, 100 and 1,500 kPa.

The SWRC software program (Dourado Neto et al., 2000) was used to fit the SWRCs using both observed and estimated data of soil moisture. The fit of each curve was evaluated based on the statistical coefficients calculated by the SWRC program. Residual moisture was considered in two forms: fixed at  $0.01 \text{ m}^3 \text{ m}^{-3}$  (Weynants et al., 2009) and variable, estimated based on the best fit of the curve.

In each situation, the S-index was obtained in five different ways. Two used observed points, with residual moisture estimated (Obs\_est) and fixed at  $0.01 \text{ m}^3 \text{ m}^{-3}$  (Obs\_001). The other three used the PTFs of Tomasella et al. (2003): for point PTF, residual moisture was also estimated (Tom\_est) and fixed at  $0.01 \text{ m}^3 \text{ m}^{-3}$  (Tom\_001); for parametric PTF, residual moisture was estimated by the model (Tom\_par).

The VGM model parameters of each curve fitted in the five ways described were entered in Eq. 2 to obtain the S-index. The S-indices of the curves relative to observed data were compared with those simulated by the curves of each type of PTF evaluated (point or parametric).

Initially, each curve fitted was evaluated based on coefficient of determination ( $R^2$ ), Akaike information criteria (AIC) and significance level (p-value) of the analysis of variance of the regression, calculated by the SWRC. AIC is a test used to differentiate models, and the smaller the difference in the AIC value, the closer the models. Only one curve of each triplicate of the conditions (management, site and layer) was selected based on these evaluations.

Observed and estimated values of S-index were statistically evaluated by linear regression through the origin. Coefficient of determination ( $R^2$ ) was estimated and Student's t-test was used to test the  $H_0$ : angular coefficient ( $\beta$ ) = 1. Significance level of 1% was adopted because of the number of observations. The modelling efficiency index (EF) recommended by Donatelli et al. (2004) to evaluate the accuracy of PTFs was also used.

## RESULTS AND DISCUSSION

The descriptive statistics of the coefficient of determination ( $R^2$ ), AIC and S-index (Table 2) was obtained as the 144 curves were fitted to the data of soil moisture and tension (observed and estimated). SWRCs obtained by Tom\_par do not have  $R^2$  and AIC, because they directly estimate the parameters of the curve, without its fitting.

Both the mean and median of the  $R^2$  relative to the fit of the observed data was higher than 0.99, expressing good fit of the curves, also confirmed by the AIC. The coefficients of

Table 2. Descriptive statistics of the coefficient of determination ( $R^2$ ), Akaike Information Criterion (AIC) and S-index for the 5 ways to obtain the soil-water retention curve (SWRC)

Obtaining of SWRC	Ind.	Mean	Statistical moments			
			Median	Max.	Min.	SD
Obs_est	$R^2$	0.994	0.998	1.000	0.967	0.008
	AIC	-16.80	-16.74	-6.03	-32.38	4.770
	S	0.038	0.037	0.099	0.009	0.020
Obs_001	$R^2$	0.993	0.996	1.000	0.962	0.007
	AIC	-16.57	-16.64	-7.92	-29.8	4.040
	S	0.030	0.029	0.077	0.009	0.012
Tom_001	$R^2$	0.986	0.989	1.000	0.935	0.012
	AIC	-10.34	-10.17	-1.41	-19.36	2.970
	S	0.044	0.042	0.133	0.022	0.017
Tom_est	$R^2$	0.990	0.996	1.000	0.947	0.013
	AIC	-10.12	-10.52	1.63	-22.20	4.130
	S	0.064	0.055	0.272	0.025	0.033
Tom_par	S	0.064	0.063	0.123	0.033	0.014

SD - Standard deviation

determination and AIC were similar between both estimates of residual moisture, with the observed data.

The means and medians of the S-index for the PTFs were higher than those of the observed data. Mean S-index values of the observed data were 0.038 and 0.030, respectively for Obs\_est and Obs\_001.

The results relative to soil moisture estimation using observed data deserve special attention. The regression of the pairs of points of the S-index between Obs\_est and Obs\_001 (Figure 2) has angular coefficient different from 1, although the coefficient of determination is higher than 0.9.

This result highlights the influence of the residual moisture determination on S-index estimate, corroborated by the observations of Jorge et al. (2010) about this moisture. In general, S-index is underestimated when residual moisture is fixed at  $0.01 \text{ m}^3 \text{ m}^{-3}$ , compared with the residual moisture estimated by the fitting.

In addition, the higher the S-index, the greater the interference of residual moisture determination on S-index. Both the mean and median of the S-index for Obs\_est were higher than the limit of quality (0.035) defined by Dexter &

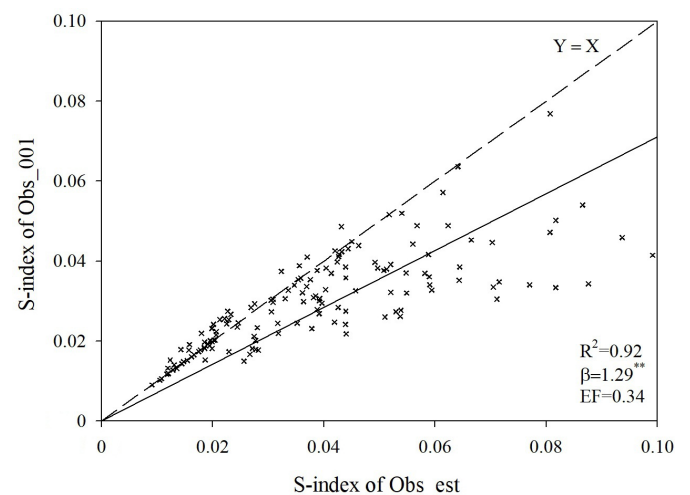


Figure 2. S-index of the observed data (144 curves), with residual moisture estimated (Obs\_est) and fixed at  $0.01 \text{ m}^3 \text{ m}^{-3}$  (Obs\_001), and regression analysis

Czyż (2007), unlike Obs\_001, which showed lower values (Table 2).

An overall trend to overestimate S-index by the PTFs was observed in the comparisons between observed and PTF-estimated data. Negative values of EF indicate inaccuracy of the estimates and, according to Donatelli et al. (2004), they indicate that the model evaluated is worse estimator than the mean of the means.

S-indices estimated by Tom\_par compared with the observed S-indices of Obs\_est and Obs\_001, along with the

regression analysis line and modeling efficiency index (EF), are presented in Figures 3A and B, respectively. The results of the point PTF of Tomasella with estimated residual moisture (Tom\_est) were also compared with the observed data, Obs\_est and Obs\_001 (Figures 4A and B).

The best coefficient of determination ( $R^2 = 0.916$ ) was found between Tom\_par and Obs\_001 (Figure 3B). However, the angular coefficient was the furthest from 1 (0.468). Besides that, all regressions between PTF-estimated and observed data

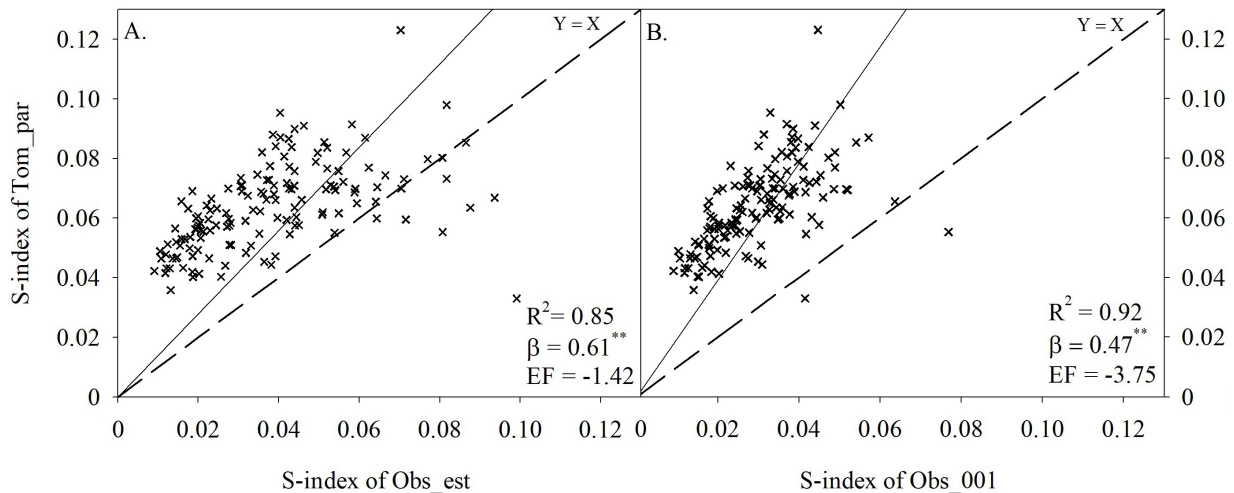


Figure 3. S-indices of the data estimated by the parametric PTF of Tomasella et al. (2003) (Tom\_par) in comparison to the observed data with residual moisture estimated (Obs\_est) (A) and fixed (Obs\_001) (B), and the regression analyses

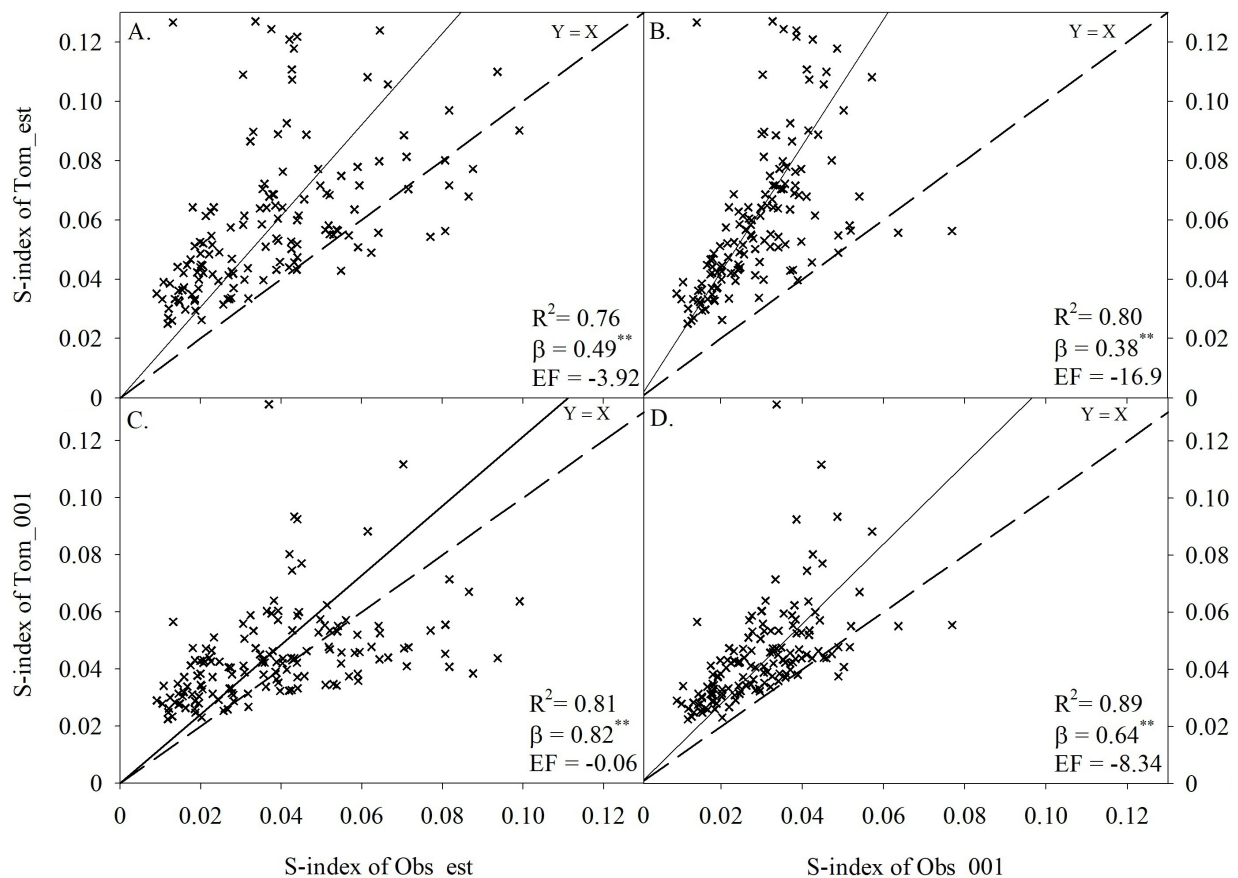


Figure 4. S-indices of the data estimated by the point PTF of Tomasella et al. (2003), in comparison to the observed data, for both residual moisture determinations. Residual moisture estimated for both, by PTF (Tom\_est) and observed data (Obs\_est) (A); Residual moisture estimated by PTF (Tom\_est) and fixed moisture in observed data (Obs\_001) (B); Fixed residual moisture on PTF (Tom\_001) and estimated with observed data (Obs\_est) (C); Fixed residual moisture for both, on PTF (Tom\_001) and observed data (Obs\_001) (D)



were significant ( $\alpha = 1\%$ ) with angular coefficient different from 1 and a variation in  $R^2$  from 0.759 to 0.895.

The regression analysis line and modeling efficiency index (EF) in the comparison between Tom\_001 and the observed data (Obs\_est and Obs\_001) are presented in Figures 4C and D, respectively. In all comparisons with the observed data, the angular coefficient was significantly different from 1. The comparison in which the angular coefficient was closest to  $\beta = 1$  was between Tom\_001 and Obs\_est ( $\beta = 0.82$ ).

Modelling efficiency index (EF) below zero in all comparisons demonstrates the difficulty of PTFs in estimating curves to predict S-index values and is probably due to several causes. First, the equation presented by Dexter (2004) to calculate the S-index (Eq. 2) depends only on 3 ( $\theta_{sat}$ ,  $\theta_{res}$  and  $n$ ) of the 5 ( $\theta_{sat}$ ,  $\theta_{res}$ ,  $m$ ,  $n$  and  $\alpha$ ) parameters of the VGM model.

The parameter “ $n$ ” is probably the most important in S-index estimation. It governs the shape of the SWRC between capillary and residual saturation (saturation zone) according to Sillers et al. (2001). The sensitivity analysis conducted by Qu et al. (2015) indicated that “ $n$ ” was the parameter that most influenced the mean water content in the soil.

The parameter “ $m$ ” governs the asymmetry of the curve close to the inflection point but becomes dependent on “ $n$ ” with the Mualem restriction. However, the scaling parameter “ $\alpha$ ” (Asgarzadeh et al., 2014) interferes with the beginning of the saturation zone. An increment in “ $\alpha$ ” changes the SWRC towards lower  $h$  values, i.e., the unsaturated zone begins at lower  $h$  values (Sillers et al., 2001).

The parameter “ $\alpha$ ” is related to the inverse of the air-entry value (Sillers et al., 2001). However, the absence of this parameter in the mathematical estimation of the S-index (Eq. 2) is probably hampering the accuracy of the estimates, evidenced by the negative values in all EF indices. Although the parameters can be related to different physical processes, the existence of interaction between processes or even between parameters should be considered.

A second cause is probably related to the estimation of residual moisture. The angular coefficient between Obs\_est and Obs\_001 was significantly different from 1 (Figure 2). Its values were also closer to 1 when residual moisture was estimated using the observed data (Obs\_est). Therefore, in the estimation of S-index, it is important that the residual moisture is not fixed because the worst EF values were obtained when it was fixed.

Jorge et al. (2010) also highlighted the importance of determining the moisture content at 1,500 kPa in the determination of the SWRC and claimed that an erroneous estimate of such moisture content could lead to incorrect results in the fit of the SWRC, as well as in the determination of S-index, emphasizing the importance of determining this moisture content in the estimation of S-index.

Asgarzadeh et al. (2014) found positive correlation of the S-index with soil available water and integral water capacity, reinforcing the importance of determining residual moisture and saturation moisture, which are extreme points of the SWRC.

The PTFs of Tomasella et al. (2003) used six inputs, four of these related to texture (contents of coarse sand, fine sand, silt and clay) and two related to structure (bulk density and

moisture equivalent); however, Dexter (2004) had already related the S-index to the structural porosity.

Working in Southern Brazil, Streck et al. (2008) related bulk density, organic matter and water available to plants to the S-index but not to the contents of clay or clay dispersed in water. Therefore, granulometry, as the main input in the PTFs evaluated, may have contributed to the inaccuracy of the estimates.

## CONCLUSIONS

1. Under field conditions in the soil diversity of the Paraná state, there were restrictions in S-index estimation using the evaluated pedotransfer functions.

2. Residual moisture should not be fixed in the fit of the SWRC to determine S-index.

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