UNIVERSIDADE FEDERAL DO PARANÁ

ALESSANDRA CALEGARI DA SILVA

AN IMPROVEMENT OF SPLINTEX: A PEDOTRANFER MODEL TO ESTIMATE SOIL HYDRAULIC FUNCTIONS

CURITIBA

2019

ALESSANDRA CALEGARI DA SILVA

AN IMPROVEMENT OF SPLINTEX: A PEDOTRANFER MODEL TO ESTIMATE SOIL HYDRAULIC FUNCTIONS

Tese apresentada ao curso de Pós-Graduação em Ciência do Solo, Setor de Ciências Agrárias, Universidade Federal do Paraná, como requisito parcial à obtenção do título de Doutor em Ciência do Solo.

Orientador: Prof. D.Sc. Robson André Armindo

CURITIBA

2019

FICHA CATALOGRÁFICA

S586a

Silva, Alessandra Calegari da
An improvment of splintex: a pedotranfer model to estimate soil hydraulic function / Alessandra Calegari da Silva. - Curitiba, 2019.
89 p.: il.,

Tese (Doutorado) - Universidade Federal do Paraná. Setor de Ciências Agrárias, Programa de Pós-Graduação em Ciências do Solo.
Orientador: Robson André Armindo

1. Ciências do Solo. 2. Solos. 3. Águas residuais no solo. I. Armindo, Robson André (Orientador). II. Título. III. Universidade federal do Paraná.

Sistema de Bibliotecas/UFPR, Biblioteca de Ciências Agrárias
Paula Carina de Araújo - CRB9/1562

TERMO DE APROVAÇÃO

MINISTÉRIO DA EDUCAÇÃO
SETOR DE CIENCIAS AGRARIAS
UNIVERSIDADE FEDERAL DO PARANÁ
PRÓ-REITORIA DE PESQUISA E PÓS-GRADUAÇÃO
PROGRAMA DE PÓS-GRADUAÇÃO CIÊNCIA DO SOLO -
40001016014P4

TERMO DE APROVAÇÃO

Os membros da Banca Examinadora designada pelo Colegiado do Programa de Pós-Graduação em CIÊNCIA DO SOLO da Universidade Federal do Paraná foram convocados para realizar a arguição da tese de Doutorado de **ALESSANDRA CALEGARI DA SILVA** intitulada: **AN IMPROVEMENT OF SPLINTEX: A PEDOTRANSFER MODEL TO ESTIMATE SOIL HYDRAULIC FUNCTIONS**, sob orientação do Prof. Dr. ROBSON ANDRÉ ARMINDO, que após após terem inquirido a aluna e realizado a avaliação do trabalho, são de parecer pela sua APROVAÇÃO no rito de defesa.

A outorga do título de doutor está sujeita à homologação pelo colegiado, ao atendimento de todas as indicações e correções solicitadas pela banca e ao pleno atendimento das demandas regimentais do Programa de Pós-Graduação.

CURITIBA, 23 de Agosto de 2019.

ROBSON ANDRÉ ARMINDO
Presidente da Banca Examinadora

LUIZ FERNANDO PIRES
Avaliador Externo (UNIVERSIDADE ESTADUAL DE PONTA GROSSA)

CEZAR FRANCISCO ARAUJO JUNIOR
Avaliador Externo (UNIVERSIDADE FEDERAL DE LAVRAS)

MARTA VASCONCELOS OTTONI
Avaliador Externo (COMPANHIA DE PESQUISA DE RECURSOS MINERAIS)

KARINA MARIA VIEIRA CAVALIERI POLIZELI
Avaliador Interno (UNIVERSIDADE FEDERAL DO PARANÁ)

ACKNOWLEDGMENT

- To my advisor, D.Sc. Robson André Armindo, for his suggestions and criticisms that contributed to the good progress of this research.
- To Dr. Celso Luiz Prevedello, who made Splintex 1.0 available, which was necessary to develop this study.
- To my supervisor in the PhD degree research abroad, Dr. Budiman Minasny, for his scientific contribution, gracious reception, and support throughout my stay in Australia.
- To the Graduate Program in Soil Science, for the opportunity of carrying out this study to obtain my PhD degree.
- To the scholarship provided by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES), for granting my PhD research.
- To the professors of the Graduate Program in Soil Science, for their valuable teachings that inspire me to continue and improve in my studies.
- To my family: my mother Maria Helena Calegari da Silva and sisters Andréia and Claudinéia Calegari da Silva, for the support and encouragement in my decisions, my nieces Gabrieli Calegari Silva, Geovanna and Melodi Calegari Rubio, thank you for everything; I love you all my little girls.
- To my boyfriend Hassan C. David, who was by my side during the great experiences and achievements of my life. Thank you for making me see life in another better way.

My best regards,

"The man is a prisoner of ignorance."

Charles Silva

RESUMO

Em busca de compreender os processos dinâmicos que ocorrem na zona vadosa, alternativas de quantificação indireta tornam-se necessárias para a estimativa das propriedades hidráulicas do solo. Uma vez que as medições dessas propriedades são muitas vezes difíceis e caras, o monitoramento em larga escala torna-se impraticável. Diante disso, neste trabalho teve-se como objetivo principal aprimorar o modelo de pedotransferência Splintex para uma segunda versão, onde os parâmetros de van Genuchten (1980)-Mualem (VGM) das funções retenção de água e condutividade hidráulica do solo foram estimados. Os resultados foram apresentados em três capítulos, que objetivaram especificamente: o desenvolvimento do algoritmo e da nova interface computacional do modelo Splintex (Splintex 2.0), comparando seu desempenho *versus* Splintex 1.0 na estimativa dos parâmetros hidráulicos para diversas classes texturais; o desempenho do Splintex 2.0, frente a dois outros modelos de pedotransferência internacionalmente reconhecidos, para estimar parâmetros da curva de retenção de água (CRA) do solo em duas extensas bases de dados de diferenciadas regiões do mundo; e o desempenho do Splintex 2.0 na estimativa da função condutividade hidráulica (CHS) do solo para diversos grupos texturais. Em relação à primeira versão, identificou-se uma pequena melhora na estimativa da CRA com o Splintex 2.0 e resultados similares aos dois modelos de pedotransferência avaliados. O Splintex 2.0 foi capaz de estimar as funções CRA e CHS, sendo a qualidade do ajuste da CHS questionável até mesmo quando realizada diretamente aos dados medidos. Como vantagem, o Splintex não requer calibração, sendo sua aplicação na estimativa da CRA e CHS de qualquer meio poroso viável.

Palavras-chave: Curva de retenção de água do solo. Condutividade hidráulica do solo. Zona vadosa. Função de pedotranferência.

ABSTRACT

In order to understand the dynamic processes that occur in the vadose zone, indirect quantification alternatives are necessary for the estimation of the soil hydraulic properties. Since measurements of these properties are often difficult and expensive, large-scale monitoring becomes impracticable. Considering the above, the main objective was to improve the Splintex pedotransfer model in a second version, where van Genuchten (1980)-Mualem (VGM) parameters from both water retention and unsaturated hydraulic conductivity functions are estimated. The results were presented in three chapters. The results were presented in three chapters, specifically: the development of the algorithm and the new computational interface of the Splintex model (Splintex 2.0), where the performance of Splintex 2.0 *versus* Splintex 1.0 in the estimation of hydraulic parameters in several textural classes was compared; the performance of Splintex 2.0, compared to two others internationally recognized pedotransfer models, to estimate soil water retention curve (SWRC) parameters in two large databases from different regions of the world; and the performance of Splintex 2.0 in the estimation of soil hydraulic conductivity (SHC) function in several textural groups. A slight improvement in the SWRC estimation with the Splintex 2.0 in relation to Splintex 1.0 was identified and results similar to the analyzed pedotransfer models. Splintex 2.0 was capable to estimate the SHC function, and the quality of this fitting was difficult even when measured data are fitted to the VGM model. As advantage, Splintex does not require calibration, allowing the estimation of SWRC and SHC for any porous medium.

Keywords: Soil water retention curve. Soil hydraulic conductivity. Vadose zone. Pedotransfer functions.

SUMMARY

1	**GENERAL INTRODUCTION**	11
1.1	OBJECTIVE	13
1.1.1	General objective	13
1.1.2	Specific objectives	13
1.2	REFERENCES	14
2	**CHAPTER I: SPLINTEX 2.0: A PHYSICALLY-BASED MODEL TO ESTIMATE WATER RETENTION AND HYDRAULIC CONDUCTIVITY PARAMETERS FROM SOIL PHYSICAL DATA**	19
2.1	ABSTRACT	19
2.2	RESUMO	20
2.3	INTRODUCTION	21
2.4	MATERIAL E METHODS	22
2.4.1	Soil hydraulic parameters	22
2.4.2	Development of PTFs to estimate soil hydraulic functions	23
2.4.3	Development environment and graphic interface of the Splintex 2.0 model	26
2.4.4	Data set and soil hydraulic parameters	28
2.5	RESULTS AND DISCUSSION	29
2.5.1	Splintex 2.0 model	29
2.5.2	Performance of the Splintex 2.0 model to estimate the hydraulic parameters	30
2.5.3	The performance of Splintex 1.0 *versus* Splintex 2.0 for the SWRC estimation	32
2.5.4	The performance of Splintex 2.0 in the estimation of hydraulic conductivity curve	35
2.6	CONCLUSIONS	38
2.7	REFERENCES	38
3	**CHAPTER II: SPLINTEX 2.0: IMPROVING A PHYSICO-EMPIRICAL MODEL FOR ESTIMATING PARAMETERS OF THE SOIL WATER RETENTION CURVE**	42
3.1	ABSTRACT	42
3.2	RESUMO	43
3.3	INTRODUCTION	44
3.4	MATERIAL E METHODS	45
3.4.1	Data set and soil hydraulic parameters	45
3.4.2	Splintex 2.0	47
3.4.3	Comparing the performance of Splintex 2.0 with other PTFs	50
3.4.4	Performance evaluation criteria	50
3.5	RESULTS AND DISCUSSION	51
3.5.1	Summary statistics of data sets used in this study	51
3.5.2	The Splintex 2.0 model	52
3.5.3	The performance of Splintex 2.0 against three PTFs	53
3.5.4	Parameters distribution	58

3.5.5	Evaluation of the water content at field capacity	60
3.6	CONCLUSIONS	61
3.7	REFERENCES	62
4	**CHAPTER III: USING SPLINTEX 2.0 TO ESTIMATE THE SOIL HYDRAULIC CONDUCTIVITY CURVE MEASURED WITH INSTANTANEOUS PROFILE METHOD**	66
4.1	ABSTRACT	66
4.2	RESUMO	67
4.3	INTRODUCTION	68
4.4	MATERIAL E METHODS	69
4.4.1	Database	69
4.4.2	Estimation of unsaturated hydraulic conductivity	71
4.4.3	Development of PTFs to estimate unsaturated hydraulic conductivity	71
4.4.4	Performance evaluation criteria	73
4.5	RESULTS AND DISCUSSION	74
4.5.1	Splintex 2.0 model	74
4.5.2	Splintex 2.0 performance for the SHCC estimation in the near-saturation range	75
4.5.3	Estimation of SHCC under different bulk density values	77
4.6	CONCLUSIONS	81
4.7	REFERENCES	81
5	**GENERAL CONCLUSIONS**	84
	GENERAL REFERENCES	85
	APPENDIX - REGISTRATION CERTIFICATE OF THE COMPUTER PROGRAM: SPLINTEX	89

1 GENERAL INTRODUCTION

In order to minimize the limitations in the study of water, air and solutes in the vadose zone of the soil, researchers have developed models with statistical and empirical (regression) or physically-grounded bases (Silva et al., 2017a; Zhang and Schaap, 2017). These models are based on pedotransfer functions (PTFs) that aim to estimate edaphic soil properties usually difficult to measure (e.g., water retention, hydraulic conductivity, specific water capacity, and hydraulic diffusivity) from the most readily available data, such as texture, organic matter (OM), bulk density (ρ_b), particle density (ρ_p) and total porosity (ϕ) (Silva et al., 2017a; Silva et al., 2017b).

The reason for introducing the term "transfer functions" (Bouma and van Lanen, 1987) and described later as a "pedotransfer function" by Bouma (1989) was to emphasize the possible link between soil research ("pedology") and soil hydrology. Soil information such as texture, ϕ, OM, ρ_b and ρ_p have a broader meaning when related directly to the soil structure. Texture provides information about the geological origin of sediments or weathering products that vary in characteristic patterns in the landscape and ϕ corresponds to the space where the dynamic processes of air and soil solution occur (Hillel, 1972). Soil particles have different shape, arrangement and structure, thus varying the relative volume of pores in the soil (macro and microporosity). However, some soils originate significantly larger values of ρ_b than others, which usually increase with soil depth unless soil compaction occurs (Prevedello and Armindo, 2015). OM is often concentrated at the soil surface and decreases characteristically in different patterns with depth for different soil types, landscapes and climate (Pachepsky and Rawls, 2004).

Simple soil information obtained through soil surveys have been established in many countries and therefore it provides an attractive source of soil data that can be used for PTFs. Thus, large databases such as Hydrophysical Database for Brazilian Soils - HYBRAS (Ottoni et al., 2018), Unsaturated Soil Hydraulic Database - UNSODA (Nemes et al., 2001), Hydraulic Properties of European Soils - HYPRES (Wösten et al., 1999), World Inventory of Soil Emission Potentials - WISE (Batjes, 1996) and Grenoble Catalogue of Soils - GRIZZLY (Haverkamp et al., 1997) are used for the purposes of the development, calibration and validation of PTFs.

Considering the close relationship between these variables, several reviews on the development and use of PTFs were published (e.g., Rawls et al., 1991; Van Genuchten and Leij, 1992; Timlin et al., 1996; Pachepsky et al., 1999; Wösten et al., 2001; McBratney et al., 2002; Vereecken et al., 2010; Botula et al., 2014; Silva and Armindo, 2016; Zhang and Schaap, 2019).

In Brazil, the first attempts to estimate available water were presented by Arruda et al. (1987), which were based on the correlation with the soil texture of the region of São Paulo. These attempts have subsidized new studies of PTFs, which have been increasing, starting with point, class and parametric principles by several researchers, such as Gaiser et al. (2000), Tomasella et al. (2000), Giarola et al. (2002), Oliveira et al. (2002), Hodnett and Tomasella (2002), Tomasella et al. (2003), Tomasella et al. (2004), Fidalski and Tormena (2007), Silva et al. (2008), Reichert et al. (2009), Michelon et al. (2010), Nebel et al. (2010), Barros et al. (2013), Medeiros et al. (2014), Medrado and Lima (2014), Soares et al. (2014) and Ottoni et al. (2019), among others, developed or used PTFs to estimate water retention data, using regression models that correlate soil physical and chemical variables, mainly texture, ρ_b and OM.

Regarding international studies, some examples in literature about the development and application of PTFs in different global zones are Schaap et al. (2001), McBratney et al. (2002), Pachepsky and Rawls, (2003); Minasny et al. (2004); Pachepsky et al. (2006); Mermoud and Xu (2006), Manyame et al. (2007), Lamorski et al. (2008), Weynants and Vereecken (2009), Ghanbarian-Alavijeh et al. (2010), Minasny and Hartemink (2011), Botula et al. (2012), Botula et al. (2013), Xiangsheng et al. (2013), Haghverdi et al. (2014), Zhang and Schaap (2017). These researches reveal the fact that PTFs are empirical in nature, forcing researchers to develop site-specific PTFs for different applications.

Pachepsky and Rawls (2004) highlighted important points about the development and application of PTFs. These authors emphasize that the apparent ease in the development of PTFs through the application of statistical regressions should not exclude the need of answering basic remaining questions about PTFs, including: *Why do PTFs exist? How to assess the reliability of PTFs? How to quantify the accuracy and reliability of PTFs? Will a grouping of soils by some criterion enhance both the accuracy and the reliability of PTFs? Is there a limit of accuracy and reliability of PTFs and what does this limit depend on? What are the most appropriate techniques to evaluate a PTF? What input variables are more preferable or necessary to be included in a PTF?* These questions can contribute to the development and advancement of PTFs in soil science.

PTFs can contribute significantly for estimating soil hydraulic functions, overcoming the difficulties of measurements, and allowing global monitoring of processes involved in the soil-plant-atmosphere interaction. In addition, PTFs become a constant reality in the scientific environment if taken into account their applicability with easily measurable and physically-grounded models for the quantification of soil hydraulic processes.

1.1 OBJECTIVE

1.1.1 General objective

To improve the algorithm of the Splintex model for estimating the parameters of the soil hydraulic functions based on physical principles.

1.2.2 Specific objectives

- To develop a new version of Splintex (Splintex 2.0), written in C++ language, with friendly interface;
- To compare the performance of Splintex 2.0 with two known-worldwide PTFs for the estimation of the soil water retention curve;
- To develop a methodology for Splintex to estimate the soil hydraulic conductivity curve;
- To compare the performance of Splintex 2.0 *versus* Splintex 1.0 for different soils around the world.

The analyses and results obtained in this work were organized and presented in three chapters:

Chapters I - Splintex 2.0: A physical-based model to estimate water retention and hydraulic conductivity functions with soil physical data;

Chapters II - Splintex 2.0: Improving a physico-empirical model for estimating parameters of the soil water retention curve;

Chapter III - Using Splintex 2.0 to estimate the soil hydraulic conductivity curve measured with instantaneous profile method.

1.2 REFERENCES

Arruda, F.B., Zullo, J., Oliveira, J.B., 1987. Parâmetros de solo para o cálculo da água disponível com base na textura do solo. **Revista Brasileira de Ciência do Solo**. 11, 11–15.

Batjes, N.H., 1996. Development of a world data set of soil water retention properties using pedotransfer rules. **Geoderma**. 71, 31–52.

Barros, A.H.C., Van Lier, Q.J., Maia, A.H.N., Scarpare, F.V., 2013. Pedotransfer functions to estimate water retention parameters of soils in northeastern brazil. **Revista Brasileira de Ciência do Solo**. 37:379–391.

Bouma, J., van Lanen, H.A.J., 1987. Transfer functions and threshold values: from soil characterisctics to land qualities. In: Proc. of the Int. **Workshop on Quantified Land Evaluation Procedures**, Washington, DC, USA, pp. 106–110.

Bouma, J., 1989. Using soil survey data for quantitative land evaluation, 1989. **Advances in Soil Science**. 9, 177–213.

Botula, Y.D., Cornelis, W.M., Baert, G., van Ranst, E., 2012. Evaluation of pedotransfer functions for predicting water retention of soils in Lower Congo (D.R. Congo). **Agricultural Water Management**.111, 1–10.

Botula, Y.D., Nemes, A., Mafuka, P., van Ranst, E., Cornelis, W.M., 2013. Prediction of water content of soils from the humid tropics by the non-parametric k-Nearest Neighbor approach. **Vadose Zone Journal**. 12, 1–20.

Botula, Y.D. Ranst, E.V., Cornelis, W.M., 2014. Pedotransfer functions to predict water retention for soils of the humid tropics: a review. **Revista Brasileira de Ciência do Solo**. 38, 679–698.

Fidalski, J., Tormena, C.A., 2007. Funções de pedotransferência para as curvas de retenção de água e de resistência do solo à penetração em sistemas de manejo com plantas de cobertura permanente em citros. **Ciência Rural**. 37, 1316–1322.

Gaiser, T., Graef, F., Cordeiro, J.C., 2000. Water retention characteristics of soils with contrasting clay mineral composition in semi-arid tropical regions. **Australian Journal of Soil Research**. 38, 523–526.

Giarola, N.F.B., Silva, A.P., Imhoff, S., 2002. Relationships between physical soil properties and characteristics of south Brazilian soil. **Revista Brasileira de Ciência do Solo**. 26, 885–893.

Ghanbarian-Alavijeh, B., Liaghat, A., Huang, G.H., van Genuchten, M.TH., 2010. Estimation of the van Genuchten soil water retention properties from soil textural data. **Pedosphere**. 20, 456–465.

Haverkamp, R.C., Zammit, F., Bouraoui, K., Rajkai, J.L.A., Heckman, N., 1997. GRIZZLY, Grenoble Soil Catalogue. Soil survey of field data and description of particle size, soil water retention and hydraulic conductivity functions. **Laboratoire d'Étude des Transfers en Hydrologie et Environnement**, LTHE, UMR5564, CNRS, INPG, ORSTOM, UJF, BP 53, 38041 Grenoble Cédex 09, xz France.

Haghverdi, A., Öztürk, H.S., Cornelis, W.M., 2014. Revisiting the pseudo continuous pedotransfer function concept: Impact of data quality and data mining method. **Geoderma**. 227, 31–38.

Hodnett, M.G., Tomasella, J., 2002. Marked differences between van Genuchten soil water-retention parameters for temperate and tropical soils: a new water-retention pedotransfer function developed for tropical soils. **Geoderma**. 108,155–180.

Hillel, D. 1971. Soil and water: Physical principles and processes. **Academic Press**, New York.

Lamorski, K., Pachepsky, Y., Slawihski, C., Walczak, R.T., 2008. Using support vector machines to develop pedotransfer functions for water retention of soils in Poland. **Soil Science Society of America Journal**. 72, 1243–1247.

Manyame, C., Morgan, C.L., Heilman, J.L., Fatondji, D., Gerard, B., Payne, W.A., 2007. Modeling hydraulic properties of sandy soils of Niger using pedotransfer functions. **Geoderma**. 141, 407–415.

McBratney, A.B., Minasny, B., Cattle, S.R., Vervoort, R.W., 2002. From pedotransfer functions to soil inference systems. **Geoderma**. 109:41–73.

Medeiros, J.C., Cooper, M., Rosa, J.D., Grimaldi, M., Coquet, Y., 2014. Assessment of pedotransfer functions for estimating soil water retention curves for the amazon region. **Revista Brasileira de Ciência do Solo**. 38, 730–743.

Medrado, E., Lima, J.E.F.W., 2014. Development of pedotransfer functions for estimating water retention curve for tropical soils of the Brazilian savanna. **Geoderma Regional**. 1, 59–66.

Mermoud, A., Xub, D., 2006. Comparative analysis of three methods to generate soil hydraulic functions. **Soil Tillage Resource**. 87, 89–100.

Michelon, C.J., Carlesso, R., Oliveira, Z.B., Knies, A.E., Petry, M.T., Martins, J.D., 2010. Funções de pedotransferência para estimativa da retenção de água em alguns solos do Rio Grande do Sul. **Ciência Rural**. 40, 848–853.

Minasny, B., Hopmans, J.W., Harter, T., 2004. Neural networks prediction of soil hydraulic functions for alluvial soils using multistep outflow data. **Soil Science Society of America Journal**. 68, 417–429.

Minasny, B., Hartemink, A.E., 2011. Predicting soil properties in the tropics. **Earth-Science Reviews**.106, 52–62.

Nebel, A.L.C., Timm, L.C., Cornelis, W., Gabriels, D., Reichardt, K., Aquino, L.S., Pauletto, E.A., Reinert, D.J., 2010. Pedotransfer functions related to spatial variability of water retention attributes for lowland soils. **Revista Brasileira de Ciência do Solo**. 34, 669–680.

Nemes, A., Schaap, M.G., Leij, F.J., Wosten, J.H.M., 2001. Description of the unsaturated soil hydraulic database UNSOSA version 2.0. **Journal Hydrology**. 251, 151–162.

Oliveira, L.B., Ribeiro, M.R., Jacomine, P.K.T., Rodrigues, J.J.V., Marques, F.A., 2002. Funções de pedotransferência para predição da umidade retida a potenciais específicos em solos do estado de Pernambuco. **Revista Brasileira de Ciência do Solo**. 26, 315–323.

Ottoni, M.V., Ottoni, F.T.B., Schaap, M.G., Lopes-Assad, M.L.R.C., Rotunno, F.O.C., 2018. Hydrophysical database for Brazilian soils (HYBRAS) and pedotransfer functions for water retention. **Vadose Zone Journal**. 17, 1–17.

Ottoni, M.V., Ottoni, T.B., Lopes-Assad, M.L.R.C., Rotunno, O.C., 2019. Pedotransfer functions for saturated hydraulic conductivity using a database with temperate and tropical climate soils. **Journal of Hydrology**. 1–35.

Pachepsky, Ya., Rawls, W.J., Timlin, D.J., 1999. The current status of pedotransfer functions: their accuracy, reliability, and utility in field- and regional-scale modeling. In: Corwin, D.L., Loague, K., Ellsworth, T.R. (Eds.), Assessment of non-point source pollution in the vadose zone, Geophysical monograph 108. **American Geophysical Union**, Washington, DC, pp. 223–234.

Pachepsky, Y.A., Rawls, W.J., 2003. Soil structure and pedotransfer functions. **European Journal Soil Science**. 54, 443–451.

Pachepsky, Y.A., Rawls, W.J., 2004. Development of pedotransfer functions in soil hydrology. New York, **Elsevier**, (Developments in Soil Science, 30).

Pachepsky, Y.A., Rawls, W.J., LIN, H.S., 2006. Hydropedology and pedotransfer functions. **Geoderma**. 131, 308–316.

Prevedello, C.L., Armindo, R.A., 2015. Física do solo: com problemas resolvidos. 2.ed. **Rev. e ampl**. Curitiba, 474p.

Rawls, W.J., Gish, T.J., Brakensiek, D.L., 1991. Estimating soil water retention from soil physical properties and characteristics. **Advances Soil Science**. 16, 213–234.

Reichert, J.M., Albuquerque, J.A., Kaiser, D.R., Reinert, D.J., Urach, F.L., Carlesso, R., 2009. Estimation of water retention and availability in soils of Rio Grande do Sul. **Revista Brasileira de Ciência do Solo**. 33, 1547–1560.

Schaap, M.G., Leij, F.J., Van Genuchten, M.Th., 2001. Rosetta: a computer program for estimating soil hydraulic parameters with hierarchical pedotransfer functions. **Journal Hydrology**. 251, 163–176.

Silva, A.P., Tormena, C.A., Fidalski, J., Imhoff, S., 2008. Pedotransfer functions for the soil water retention and soil resistance to penetration curves. **Revista Brasileira de Ciência do Solo**. 32, 11–19.

Silva, A.C., Armindo, R.A., 2016. The importance of pedotransfer functions to study the hydraulic properties in Brazilian soils. **Multi-Science Journal**. 5, 31–37.

Silva, A.C., Armindo, R.A., Brito, A.S., Schaap, M.G., 2017a. Splintex: A physically-based pedotransfer function for modeling soil hydraulic functions. **Soil Tillage Resource**. 174, 261–272.

Silva, A.C., Armindo, R.A., Brito, A.S., Schaap, M.G., 2017b. An assessment of pedotransfer function performance for the estimation of spatial variability of key soil hydraulic properties. **Vadose Zone Journal**. 16, 1–10.

Soares, F.C., Robaina, A.D., Peiter, M.X., Russi, J.L., Vivan, G.A., 2014. Redes neurais artificiais na estimativa da retenção de água do solo. **Ciência Rural**. 44, 293–300.

Timlin, D.J., Pachepsky, Ya., Acock, B., Whisler, F., 1996. Indirect estimation of soil hydraulic properties to predict soybean yield using GLYCIM. **Agricultural Systems**. 52, 331–353.

Tomasella, J., Hodnett, M.G., Rossato, L., 2000. Pedotransfer functions for the estimation of soil water retention in Brazilian soils. **Soil Science Society of America Journal**. 64, 327–338.

Tomasella, J., Pachepsky, Y., Crestana, S., Rawls, W.J., 2003. Comparison of two techniques to develop pedotransfer functions for water retention. **Soil Science Society of America Journal**. 67, 1085–1092.

Tomasella, J., Hodnett, M.G., 2004. Pedotransfer functions for tropical soils. In: Pachepsky, Y.A. and Rawls, W.J., ed. Development of pedotransfer functions in soil hydrology. Amsterdam, **Elsevier**, p. 415–429.

Van Genuchten, M.Th., Leij, F., 1992. On estimating the hydraulic properties of unsaturated soils. In: van Genuchten, M. Th., Leij, F.J., Lund, L.J. (Eds.), Indirect Methods for Estimating the Hydraulic Properties of Unsaturated Soils. University of California, **Riverside**, CA, pp. 1–14.

Vereecken, H., Weynants, M., Javaux, M., Pachepsky, Y., Schaap, M.G., Van Genuchten, M.Th., 2010. Using pedotransfer functions to estimate the van Genuchten-Mualem soil hydraulic properties: a review. **Vadose Zone Journal**. 9,1–26.

Xiangsheng, Y., Guosheng, L., Yanyu, Y., 2013. Comparison of three methods to develop pedotransfer functions for the saturated water content and field water capacity in permafrost region. **Cold Regions Science and Technology**. 88, 10–16.

Weynants, M., Vereecken, H., Javaux, M., 2009. Revising Vereecken pedotransfer functions: Introducing a closed-form hydraulic model. **Vadose Zone Journal**. 8, 86–95.

Wösten, J.H.M., Lilly, A., Nemes, A., Le Bas, C., 1999. Development and use of a database of hydraulic properties of European soils. **Geoderma**. 90, 169–185.

Wösten, J.H.M., Pachepsky, Ya., Rawls, W.J., 2001. Pedotransfer functions: bridging the gap between available basic soil data and missing soil hydraulic characteristics. **Journal Hydrology**. 251, 123–150.

Zhang, Y., Schaap, M., 2017. Weighted recalibration of the Rosetta Pedotransfer model with improved estimates of hydraulic parameter distributions and summary statistics (Rosetta3). **Journal Hydrology**. 547, 39–53.

Zhang, Y., Schaap, M., 2019. Estimation of saturated hydraulic conductivity with pedotransfer functions: A review. **Journal Hydrology**. 575, 1011–1030.

2 CHAPTER I: SPLINTEX 2.0: A PHYSICALLY-BASED MODEL TO ESTIMATE WATER RETENTION AND HYDRAULIC CONDUCTIVITY PARAMETERS FROM SOIL PHYSICAL DATA

2.1 ABSTRACT

Soil water retention curve (SWRC) and hydraulic conductivity curve (SHCC) are functions that contribute to the understanding and modeling of hydraulic processes in the vadose zone of the soil. However, their measurement is often difficult and expensive becoming impractical the large-scale monitoring. Pedotransfer functions (PTFs) are, therefore, an alternative to estimate SWRC and SHCC data. Most PTFs are usually calibrated with data from local soils and may be uncertain when applied to soils with different morphological properties. On the other hand, PTFs with a physico-empirical basis have as advantage their wide application. Splintex 1.0 is a physico-empirical model developed in BASIC language that is based on the particle size distribution and other basic soil information. This model estimates the parameters of the van Genuchten-Mualem equation that compose the SWRC without requiring prior calibration and the saturated hydraulic conductivity (K_s) using a texture-PTF. A second version with a user-friendly computational interface is presented to improve the estimates of the SWRC parameters and to introduce the estimation of the SHCC parameters with different PTFs, which are based on two physically-based models that can be applied universally. Computational procedures and equations of Splintex 2.0 were written in C ++ language and the performance of both model versions was tested for different soil texture classes. The performance analysis was carried out using the Pearson correlation coefficient and the mean absolute and root mean square errors. Splintex 2.0 yielded good performance in the quantification of water retention data, showing its application to any soil class. As an advantage, the conductivity data can be estimated without the need of K_s and SWRC parameters.

Keywords: Soil water retention curve; soil hydraulic parameters; pedotransfer function; particle size distribution.

2.2 RESUMO

A curva de retenção de água (CRA) e a condutividade hidráulica do solo (CH) são funções que contribuem para o entendimento e modelagem dos processos hidráulicos na zona vadosa do solo. No entanto, suas medidas são muitas vezes difíceis e caras, tornando-se impraticáveis o monitoramento em larga escala. As funções de pedotransferência (FPTs) são uma alternativa para estimar tanto CRA quanto a CH. Geralmente, as FPTs são calibradas a partir de solos de áreas locais, sendo incertas quando aplicadas em solos com diferentes propriedades morfológicas. Por outro lado, FPTs fisicamente fundamentadas acabam sendo vantajosas em termos de utilização. O Splintex 1.0 é um modelo físico-empírico desenvolvido na linguagem BASIC, baseado na distribuição do tamanho de partículas e outras informações físicas do solo. Este modelo estima os parâmetros CRA da equação de van Genuchten-Mualem sem necessitar de calibração prévia, e a condutividade hidráulica saturada (*Ks*) usando uma FPT com base textural. Uma segunda versão com uma interface computacional amigável é apresentada para melhorar as estimativas dos parâmetros da CRA e introduzir a estimativa dos parâmetros da CH com diferentes FPTs, que são baseadas em dois modelos físicos que podem ser aplicados universalmente. Os procedimentos e equações computacionais do Splintex 2.0 foram escritos em linguagem C ++ e o desempenho de ambas versões foram testados para diferentes classes texturais. A análise de desempenho foi realizada utilizando o coeficiente de correlação Pearson, erro médio absoluto e raiz quadrada do erro médio. O Splintex 2.0 apresentou bom desempenho na quantificação da retenção de água, mostrando sua aplicação em qualquer classe de solo. Como vantagem, os dados de condutividade podem ser estimados sem a necessidade dos parâmetros K_s e CRA.

Palavras-chave: Curva de retenção de água no solo. Parâmetros hidráulicos do solo. Função de pedotransferência. Distribuição de tamanho de partícula.

2.3 INTRODUCTION

Whatever the scale applied, soils are intrinsically heterogeneous and this heterogeneity controls their hydraulic behavior (Vogel and Roth, 2003; Weynants et al., 2009). The soil water retention curve [SWRC, $\theta(h)$] and soil hydraulic conductivity curve [SHCC, $K(\theta)$] are functions that predict hydraulic processes in the vadose zone. The quest to improve and develop methods to quantify and analyze soil hydraulic functions in different morphology, hydrology and climate conditions is a crucial topic in soil science research.

In an attempt to minimize the limitations in the study of water in the vadose zone, researchers have developed empirical or physically-based pedotransfer functions (PTFs). PTFs are applied in the estimation of the soil hydraulic data in an indirect way, relying on more readily available data (e.g., texture, soil organic carbon and bulk density). The term PTF was first introduced by Bouma (1989), who aimed to unify various terms used in the literature to describe the meaning of transforming existing information into nonexistent data.

The main supposition that underlies most PTFs is that textural properties dominate the hydraulic behavior of soils (Tomasella et al., 2008; Botula et al., 2012; Haghverdi et al., 2014; Silva et at., 2017a; Karup et al., 2017). There are limitations of some texture-PTFs available in the literature because of the non-incorporation of any soil structural property. It is well-known that structural information has influence on the soil hydraulic behavior (Weynants et al., 2009) and they are crucial for a better description of the wet range of both water retention and hydraulic conductivity curves.

The reliability of PTFs applied in a geographic region different from the one for where they were originally developed is often limited due to geological, hydrological, climatic and land use factors. An alternative for overcoming the inherent empiricism is the development of PTFs based on physical considerations. Thus, in the last two decades, the search for models based on physical concepts has been focused on finding a tool to estimate hydraulic parameters via PTFs. In addition, the current computer performance allows the use of global search algorithms, which can improve the estimation of hydraulic parameters and therefore the development of PTFs.

Based on these considerations, we aimed to improve Splintex 1.0 for the estimation of water retention and conductivity parameters. Splintex 1.0 is a physically-based model developed by Prevedello and Loyola (2002) in a computer program language (BASIC) to estimate the parameters of van Genuchten (1980)-Mualem, hereafter abbreviated as VGM. In this first version, Splintex also estimates the saturated hydraulic conductivity (K_s) according to the measured data set of Rodas (1970). This computer program applies a simplification of the

Arya and Paris (1981) model (AP) to convert particle size distribution (PSD) data into total porosity, fraction of solid mass and then into soil water content (θ) and soil water tension (h). Because it is a physically-based model, Splintex can be applied to any porous medium without the need of calibration (Silva et al., 2017a).

As reported by Reis et al. (2018), Splintex 1.0 presents in its structure two main PTFs that require as input data texture and bulk and particle densities. Notably, the second PTF also requires the saturated water content and any other measured $\theta(h)$ point to improve the estimation. Some other PTFs require specific $\theta(h)$ points for running their estimations.

The model Splintex 1.0 has been used by Brazilian researchers in soil mass balance, physical quality and irrigation studies (Prevedello et al., 2007; Souza and Gomes, 2008; Scussiato, 2012; Reis et al., 2018). However, its goodness-of-fit was only systematically evaluated when Silva et al. (2017a) described its estimates for 103 SWRCs, when it was applied to simulate the spatial variation of soil hydraulic properties (Silva et al., 2017b) and when its two-main PTFs were analyzed for 50 SWRCs for Brazilian soils (Reis et al., 2018).

The initial interest in developing a new version of Splintex was due to its obsolete BASIC language, the fact is that it could neither read nor export the results. Furthermore, it did not provide even the possibility of running more than one SWRC at the same time. Another motivation was the need of enhancing its algorithm code in order to improve the estimation of the function $\theta(h)$ and to create the estimation of the function $K(\theta)$. Silva et al. (2017a) commented that the values of θ_s and K_s estimated with Splintex 1.0 overestimated the results measured for soils of several Brazilian regions. Therefore, the first version led us to consider whether the model should be improved, contributing to the understanding of the soil-water relationship and providing subsidies for new research with lower costs.

The objectives in this study were to develop a new computational interface of the Splintex model (Splintex 2.0), to improve the algorithm of the Splintex to estimate the soil hydraulic parameters and to evaluate the estimation performance of Splintex 2.0 *versus* Splintex 1.0 for different soil textural classes.

2.4 MATERIAL AND METHODS

2.4.1 Soil hydraulic parameters

Splintex 2.0 is a computer program able to estimate van Genuchten (1980)-Mualem (VGM) parameters from both water retention and unsaturated hydraulic conductivity functions.

The equation to describe the soil water retention function is given by

$$\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{\left[1 + (\alpha \cdot h)^n\right]^{1-1/n}} \tag{1}$$

in which θ is the volumetric soil water content ($m^3\ m^{-3}$) as a function of the soil water tension (h), with $h > 0$ for unsaturated conditions (m), θ_r and θ_s are respectively the residual and saturated water content ($m^3\ m^{-3}$), α (m^{-1}), n and m (m=1-1/n) are empirical curve shape factors. In this study, h is defined as the modulus of matric potential and expressed in units of energy per weight (m =J/N).

Deriving the restriction described by Mualem (1976), m=1-1/n, van Genuchten (1980) yielded the following closed-form expression for the unsaturated hydraulic conductivity:

$$K(\theta) = K_s \Theta^{\lambda}\left[1-\left(1-\Theta^{1/m}\right)^m\right]^2 \tag{2}$$

in which the effective saturation (Θ), is computed as

$$\Theta = \frac{\theta - \theta_r}{\theta_s - \theta_r} \tag{3}$$

and K_s is a fitted matching point at saturation (cm d^{-1}) and λ an empirical parameter related with the connectivity of pores.

2.4.2 Development of PTFs to estimate soil hydraulic functions

The AP model presents in its structure a set of physical equations to quantify data pairs of θ and h. The calculation of θ is taken from the particle size distribution (PSD), as a contribution of each fraction to soil wetting, according to:

$$\theta_i \approx \phi S_w \sum_{j=0}^{j=i} w_j; \quad i = 1, 2, ..., n \tag{4}$$

in which ϕ is the total porosity of the soil sample ($m^3\ m^{-3}$), S_w is the ratio of measured saturated water content to theoretical porosity and w_i is the solid mass of the i-th fraction (kg kg^{-1}).

The second principle is the capillarity equation that relates h to the radius of the largest pore filled with water (R_i). The value of R_i is estimated using the particle size class and a scale factor (β) for correcting the possible non-sphericity of the soil particles (Arya and Paris, 1981; Arya et al., 1999a). The combination of R_i and h results in:

$$h_i \approx \frac{2\,\sigma\,cos\,(\omega)}{\rho_w g \mu_i \sqrt{\dfrac{2(\rho_p - \rho_b)}{3\rho_b}\left(\dfrac{3w_i}{4\pi\mu_i^3\rho_p}\right)^{1-\beta}}}; \qquad i = 1,\, 2,\, \ldots, n \tag{5}$$

in which σ is the coefficient of surface tension at the air–water interface (kg s^{-2}), μ is the soil particle radius, considering packing of spherical particles (m), ω is the contact angle in the largest water-filled pore (AP model considers ω=0), w_i is the solid mass of the i-th fraction (kg kg^{-1}), g is gravity (m s^{-2}), ρ_w is the density of water (kg m^{-3}), ρ_b and ρ_p are the soil bulk and particle density (kg m^{-3}), respectively. A more complete description to obtain equation 5 is given in Arya and Paris (1981).

The constant value of $\beta = 1.38$ suggested by AP model worked well for some soils, but not for all PSDs. Arya et al. (1982) analyzed 181 soil samples from New Jersey and found values of $1.26 \leq \beta \leq 2.10$. Vaz et al. (2005) reported an average value of $\beta = 0.977$ for 104 soil samples obtained from the Southern and Southeastern Brazil.

For both Splintex 1.0 and 2.0, 1.20 is an initial value used for β. Unless the volume fraction of solids (the ratio of the volume of solid particles to the total volume of soil) is smaller than 7.6% and the sum of the percentage of particles of 0.1-mm diameter is smaller than 60%, β is then assumed to be 1.15. However, when this sum of the percentage of particles is larger than 60%, $\beta = 1.0$. For other values of volume fraction of solids and distribution of particles of 0.1-mm diameter, β is assumed as a function of h (Arya et al., 1999a):

$$\beta = 1 - \frac{log_{10}\left[\dfrac{3}{2e}\left(2\sigma/\rho_w g h_i \mu_i\right)^2\right]}{log_{10}\left(3w_i/4\pi\mu_i^3\rho_p\right)} \tag{6}$$

in which e is the void ratio (volume of voids/volume of particles), given by $e = (\rho_p - \rho_b)/\rho_b$. Thereby, using the measured $\theta(h)$ point informed by the user, Splintex 2.0 combines equations 5 and 6 to calculate β.

Because the aim is the size and distribution of pores and not the size and distribution of particles, some deviations may occur in this estimation. They can be minimized if the user provides one (θ_s) or two [θ_s and any other $\theta(h)$ value] experimental points on the retention curve.

Otherwise, an automatic correction to estimate $\theta(3.3\ m)$ is accomplished with another PTF, presented by Arruda et al. (1987):

$$\theta(3.3m)= 7.00138\rho_b\, exp\left[3.9\times10^{-2}(\%Clay+\%Silt)-2.6\times10^{-4}(\%Clay+\%Silt)^2\right] \quad (7)$$

in which $\theta(3.3\ m)$ is the soil water content ($m^3\ m^{-3}$) at the water tension of 3.3 m and ρ_b is the bulk density (kg dm^{-3}). Inasmuch as the value β is quantified, Splintex 2.0 estimates the SWRC parameters fitting θ and h data obtained with equations 4 and 5, respectively.

Regarding the SHCC data, we used a compilation of the methodologies proposed by Arya et al. (1981), Arya et al. (1999b) and Arya et al. (2015) for the unsaturated hydraulic conductivity [$K(\theta)$] estimation. Splintex 2.0 model is based on the assumption that the soil pores can be represented by equivalent capillary tubes and that the flow rate (q) is a function of pore size distribution (Arya et al., 1999b). Therefore, $K(\theta)$ is computed by

$$K(\theta_i)=\frac{1}{A_b}\sum_{j=1}^{j=i}\left(cR_j^x\right)N_j\ ;\quad i = 1,2,...,n \quad (8)$$

in which N_j is the number of pores in the i-th pore fraction, exposed at the cross-sectional area, R_j is the pore radius i-th fraction (m), A_b is the cross-sectional area (m^2) of the sample given by $A_b = (1/\rho_b)^{2/3}$ and c and x are empirical parameters described in table 1.

In this approach, the sum of the flow rates of each saturated pore of a given soil sample is computed assuming the Hagen-Poiseuille's law for capillary flow (Prevedello and Armindo, 2015). Therefore, $K(\theta)$ is computed as

$$K(\theta_i)=\frac{1}{A_b}\sum_{j=1}^{j=i}\left(q_j\right)N_j\ ;\quad i = 1,2,...,n \quad (9)$$

in which N_j is the number of pores in the i-th pore fraction exposed at the cross-sectional area, A_b is the cross-sectional area of the sample (m^2), given by $A_b = (1/\rho_b)^{2/3}$, and q_j is the volumetric flow rate for a single pore ($m^3\ s^{-1}$), calculated by $q_j=cR_j^{\ x}$. A more complete description of the $K(\theta)$ estimation is provided in Arya et al. (1999b).

Following Arya et al. (2015), the estimation of $K(\theta)$ can be improved obtaining the R_i data. The authors formulated the individual pore radius correspondent to each fraction of particles with the information usually available for most soils, by means of:

$$R_i = \sqrt{\frac{0.0717\,\phi\, w_i}{\tau_i^{4/3}\,\mu_i\,\rho_b}} \quad (10)$$

in which R_i is the pore radius for a given fraction of particles on the PSD curve (m) and τ_i is the number of spherical particles that could be formed using the fraction solid mass. Equation 10 eliminates the need of unknown empirical parameters.

2.4.3 Development environment and graphic interface of the Splintex 2.0 model

Splintex 2.0 consists of a computational algorithm developed in C++, compiled in an Integrated Programming Environment (IDE) CodeBlocks, structured with data input, mathematical interactions and data output. Splintex 2.0 presents some optional functions for estimating VGM parameters of equations 1, 2 and 3, according to the availability of input data and the user's decision of assuming θ_s as only a statistical fitting parameter or as an independent parameter with its physical meaning associated with total porosity.

As shown in figure 1, the interface of the Splintex 2.0 model was developed with an input structure, optional information and output data.

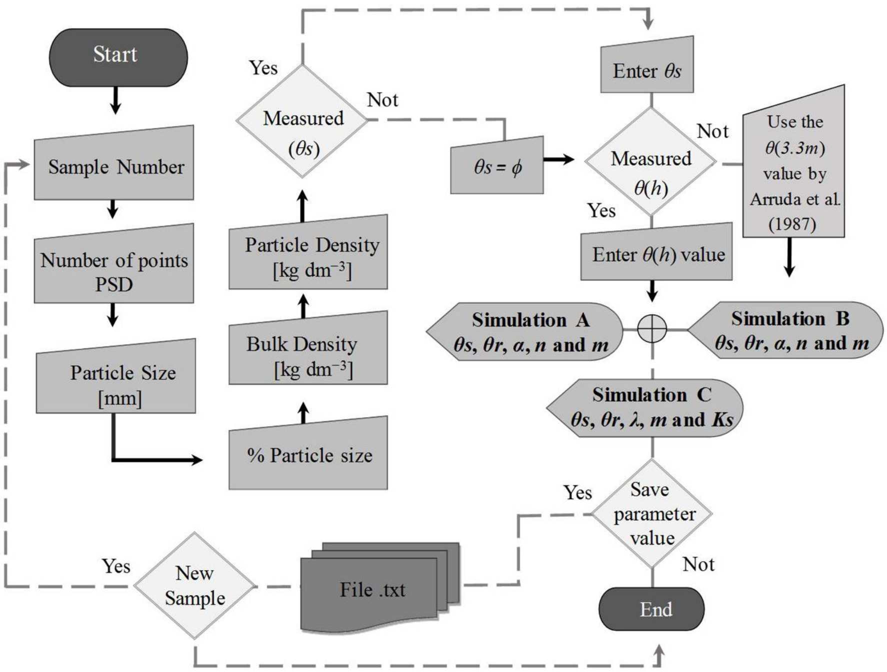

Figure 1 - Flowchart of the Splintex 2.0 algorithm. The output of the VGM parameters are presented in three ways; simulation A: θ_s was set as its measured value and θ_r, α, n and m

estimated; simulation B: all parameters θ_s, θ_r, α, n and m estimated; simulation C: all parameters θ_s, θ_r, λ, m and K_s estimated; PSD: particle size distribution.

The required inputs are:

The model requires the sample identification and the number of texture points (N) to create a dimension vector continuously stored in its memory. Each particle diameter and its equivalent percentage values are then inserted. After that, a cubic spline function is fitted to these data for describing the cumulative PSD function. Thus, we standardized PSD for 16 classes of particle diameters: 2, 4, 6, 8, 10, 20, 40, 50, 60, 80, 100, 200, 400, 600, 800 and 1000 µm within a "for" command. To finish the procedure, the values of ρ_b and ρ_p are required.

The optional inputs are:

In The measured θ_s is required and if its value is unknown the total porosity (ϕ) replaces it by $\phi = 1 - \rho_b/\rho_p$, then the algorithm proceed equations 4, 5 and 6. Some deviations in these estimation may occur due to the transformation of PSD into pore size distribution data to estimate $\theta(h)$ and $K(\theta)$ parameters. The deviations in the estimation of $\theta(h)$ parameters can be minimized if any measured $\theta(h)$ point is provided, otherwise the automatic correction presented in equation 7 is accomplished to find the best value of β (Equation 6). Thereby, the estimated $\theta(h)$ values are fitted to equation 1 and the estimated $K(\theta)$ data to equation 2 applying the non-linear regression optimization.

The estimation of the parameters of equation 1 accomplished with the two-main PTFs of Splintex was evaluated in this study. The inputs used in the first PTF (Splintex-PTF1) were PSD, ρ_b, ρ_p and θ_s whereas in the second PTF (Splintex-PTF2) PSD, ρ_b, ρ_p, θ_s and measured $\theta(h)$ point were inserted.

The output window is divided in:

• Two outputs of the parameters of equation 1 are presented. In the second column is the simulation A, where four parameters (θ_r, α, n and m) are estimated and θ_s is set to the measured θ_s or ϕ. In the third column, Simulation B results in five estimated parameters (θ_s, θ_r, α, n and m). Parameter m is calculated by $m=1-1/n$ for both simulations.

• The fourth column provides estimates of the parameters θ_s, θ_r, λ, m and K_s, described in equations 2 and 3 (Simulation C).

2.4.4 Data set and soil hydraulic parameters

The data set used in this study was obtained through the Hydrophysical Database for Brazilian Soils - HYBRAS (Ottoni et al., 2018) and the Unsaturated Soil Database - UNSODA (Nemes et al., 2001). The combined data set contains 467 samples of $\theta(h)$ and $K(\theta)$ together with their basic soil properties. This data set represented a wide range of soil textures (Table 1), in which nine textural classes are represented.

Table 1: Summary statistics for ranges of soil texture (according to USDA classification), bulk density (ρ_b), particle density (ρ_p) and total porosity (ϕ) for nine soil texture classes.

Soil texture Classes	Statistic	Fraction (% mass)			ρ_b	ρ_p	ϕ	Number of samples	Parameters	
		Sand	Silt	Clay	kg dm^{-3}		%		*log (c)*	*x*
Clayey	Mean	23.98	20.42	55.60	1.18	2.66	55.50	80	-0.488	3.506
	Maximum	43.66	39.00	88.00	1.52	3.67	68.78			
	Minimum	1.80	7.00	40.40	0.72	2.14	42.86			
	SD	12.31	9.37	10.82	0.20	0.23	7.30			
Silty clay	Mean	12.75	43.28	43.98	1.18	2.60	54.55	35	-0.488	3.506
	Maximum	18.10	51.40	51.70	1.43	2.78	64.59			
	Minimum	3.90	35.70	40.00	0.87	2.46	45.95			
	SD	4.15	3.35	2.43	0.15	0.08	5.10			
Sandy clay	Mean	50.11	9.60	40.29	1.42	2.58	44.92	67	-0.488	3.506
	Maximum	59.00	17.35	45.60	1.73	2.75	66.67			
	Minimum	45.12	5.00	35.28	0.79	2.36	33.33			
	SD	3.33	2.77	2.94	0.20	0.10	7.85			
Clayey loam	Mean	37.52	30.08	32.39	1.32	2.57	48.91	28	2.647	4.258
	Maximum	60.10	46.20	39.43	1.74	2.87	70.68			
	Minimum	21.20	16.37	14.80	0.56	1.91	32.56			
	SD	8.79	7.66	5.35	0.30	0.20	9.83			
Silty loam	Mean	4.36	71.25	24.39	1.60	2.65	43.80	41	2.647	4.258
	Maximum	15.69	84.05	33.93	1.74	2.65	51.65			
	Minimum	1.16	53.18	14.13	1.39	2.65	39.45			
	SD	3.02	6.77	5.38	0.08	0.00	2.48			
Sandy c. loam	Mean	63.65	8.88	27.47	1.56	2.57	39.42	65	0.482	3.602
	Maximum	73.00	18.00	35.00	1.84	2.75	61.13			
	Minimum	49.20	3.00	20.00	0.96	2.30	29.31			
	SD	5.73	3.15	4.29	0.17	0.09	6.04			
Loamy	Mean	44.21	40.03	15.76	1.55	2.51	38.35	45	2.647	4.258
	Maximum	50.05	44.91	26.50	1.71	2.68	55.98			
	Minimum	33.00	34.60	12.98	1.13	2.39	30.77			
	SD	3.14	2.54	2.53	0.12	0.07	5.27			
Sandy loam	Mean	70.70	14.08	15.22	1.55	2.60	40.31	53	-0.871	3.063
	Maximum	82.50	34.00	19.00	2.01	2.70	64.65			
	Minimum	52.28	2.01	7.70	0.92	2.46	24.44			
	SD	9.01	9.12	3.23	0.17	0.05	6.45			
Sandy	Mean	78.63	5.70	15.66	1.56	2.70	41.83	47	1.849	3.999
	Maximum	93.00	8.00	20.90	1.88	2.82	47.10			
	Minimum	73.17	2.00	2.00	1.45	2.59	31.11			
	SD	7.26	1.25	6.66	0.11	0.03	3.83			

Sandy c. loam: Sandy clay loam, *c* and *x*: parameters of the function $K(\theta)$ described in equation 8 and SD: standard deviation.

The performance criterion used to evaluate the Splintex estimates was executed with the following summary statistics: minimum, maximum, mean and standard deviation. As accomplished in other studies that analyzed PTFs (Zhang and Schaap, 2017; Reis et al., 2018), the goodness of fit was assessed with the Pearson correlation coefficient (*r*), mean absolute error (MAE) and root mean square error (RMSE), as follows:

$$r = \frac{Cov\left(\theta_{est}, \theta_{mea}\right)}{S_{\theta_{est}} S_{\theta_{mea}}} \tag{11}$$

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{n}\left(\theta_{est_i} - \theta_{mea_i}\right)^2} \tag{12}$$

$$MAE = \frac{1}{N}\sum_{i=1}^{n}\left|\theta_{est} - \theta_{mea}\right| \tag{13}$$

in which θ_{mea} is the *i*-th measured variable, θ_{est} is the *i*-th estimated variable, *Cov* is the covariance, *N* is the number data, $S_{\theta mea}$ and $S_{\theta est}$ are standard deviation of the measured and estimated data.

A correlation matrix with the *r* values for each estimated parameter yielded by measured data and estimated by Splintex 2.0 was done with the significance test verified by the Student's t-test at 5% probability.

2.5 RESULTS AND DISCUSSION

2.5.1 Splintex 2.0 model

The new developed version of Splintex model is shown in figure 2. In left side of the window, a box with the description of the input data is presented. The output results of the parameters of equation 1, 2 and 3 is revealed in another box at the right side of the window. At the upper left corner, the information about the system menu is organized with functions to import and export data, quit and a file with the previous published studies with Splintex 1.0.

Manually: Users can manually enter the value of each requested variable in a sequential way.

Import: This item is used to import a *.txt* file and read input variables for simulation with easy input data in sequence. For it, the button "Import File" should be triggered for choosing the *.txt* file containing the sample number and values of the diameters (mm) of the particles that compose the PSD. Textural contents (%), ρ_b and ρ_p (kg dm^{-3}) and the optional values of measured θ_s and any other $\theta(h)$ point should be filled in this file. Then, for running Splintex 2.0 model, the button "Run" should be clicked on and "Next" to a new iteration.

Export: Results of each simulation are exported in a *.txt* file. For each iteration, the estimated VGM parameters are saved clicking on "Save" button. Subsequently, users can press the "Export File" button to create a *.txt* file with the results in a folder.

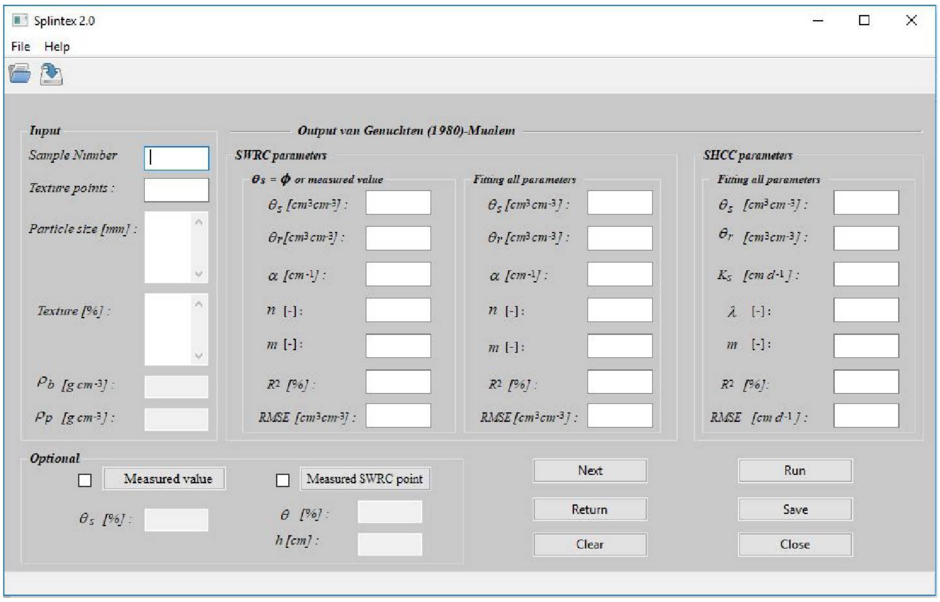

Figure 2 - Initial window of Splintex 2.0.

2.5.2 Performance of the Splintex 2.0 model to estimate the hydraulic parameters

Results of the correlations between VGM parameters estimated with Splintex 2.0 and Splintex 1.0 in this study are presented in table 2, respectively. The values of Pearson correlation (*r*) for θ_s were close amongst the six major texture groups, unlikely for Splintex 1.0-PTF1 and Splintex 1.0-PTF2 that revealed *r* values from -0.569 to 0.793 for sandy and sandy loam texture, respectively. For other estimations, *r* revealed values between 0.826 and 0.994.

The improvement for θ_s, particularly in the data with high sand content, was obtained due to the change in its constraint used in the algorithm. For Splintex 1.0, this restriction was programmed as: *if* $\theta_s > \phi$ then $\theta_s = \phi$. However, θ_s is running in Splintex 1.0 as a percentage value (%) yielding results larger than 1 ($\theta_s > 1$) for extremely sandy soils, which is not realistic. This result was not previously identified by Silva et al. (2017a), Silva et al. (2017b) and Reis et al. (2018), since their evaluated data sets were composed by soils with different textural contents of the soils evaluated in this study.

In contrast to θ_s, θ_r is just a fitting parameter, defined by van Genuchten (1980) as the water content for which h tends to the infinity. In general, all PTFs presented small values of r. However, the estimates with Splintex 2.0-PTF-simA and Splintex 2.0-PTF2-simB were more accurate for θ_r for the clayey texture, with values about 0.40 and 0.35. This small advantage of PTF1 can be explained by the use of the $\theta(h)$ point in the PTF2 estimation. Reis et al. (2018) addressed moderate correlations ($0.47 \leq r \leq 0.60$) for estimates using Splintex 1.0 for different soil textures.

Table 2: Pearson correlation for VGM parameters between measured and estimated data by Splintex 1.0 and Splintex 2.0 models for six main groups of soil texture.

Parameters	Splintex 1.0 PTF1	Splintex 1.0 PTF2	Splintex 2.0-PTF1 simA	Splintex 2.0-PTF1 simB	Splintex 2.0-PTF2 simA	Splintex 2.0-PTF2 simB
	Clayey					
θ_s ($m^3 m^{-3}$)	0.866	0.882	0.896	0.893	0.896	0.903
θ_r ($m^3 m^{-3}$)	-0.006	0.081	0.059	-0.071	0.401	0.349
α (m^{-1})	-0.065	-0.145	-0.083	-0.086	-0.149	-0.226
n	-0.363	0.314	-0.253	-0.291	0.450	0.348
	Clayey loam					
θ_s ($m^3 m^{-3}$)	0.895	0.902	0.900	0.902	0.900	0.897
θ_r ($m^3 m^{-3}$)	0.297	0.302	-0.275	0.043	0.154	0.070
α (m^{-1})	-0.383	-0.114	-0.334	-0.354	-0.058	-0.139
n	0.111	0.132	-0.164	0.123	0.395	0.244
	Silty loam					
θ_s ($m^3 m^{-3}$)	0.994	0.994	0.994	0.983	0.994	0.980
θ_r ($m^3 m^{-3}$)	0.453	0.452	-0.007	0.025	0.066	0.200
α (m^{-1})	0.139	0.535	0.095	0.156	0.248	0.224
n	-0.029	-0.093	0.351	0.123	0.075	0.027
	Sandy					
θ_s ($m^3 m^{-3}$)	-0.569	0.793	0.779	0.750	0.779	0.826
θ_r ($m^3 m^{-3}$)	0.466	0.465	0.467	0.109	0.401	0.264
α (m^{-1})	-0.054	-0.147	-0.107	-0.028	-0.041	0.025
n	0.052	-0.064	-0.035	-0.182	-0.164	0.704
	Sandy loam					
θ_s ($m^3 m^{-3}$)	0.151	0.267	0.857	0.857	0.857	0.845
θ_r ($m^3 m^{-3}$)	0.612	0.608	0.597	0.150	0.331	-0.054
α (m^{-1})	0.235	0.353	0.082	-0.027	0.073	0.209
n	-0.072	-0.040	-0.060	-0.036	0.201	0.081
	Loamy					
θ_s ($m^3 m^{-3}$)	0.876	0.871	0.878	0.877	0.878	0.868
θ_r ($m^3 m^{-3}$)	0.066	0.099	0.116	-0.080	0.159	0.135
α (m^{-1})	-0.123	0.512	-0.235	0.017	0.227	0.284
n	-0.262	-0.023	-0.046	-0.192	0.076	-0.005

θ_s: saturated water content, θ_r: residual water content, α and n: fitting parameters of equation 1, SimA: results of the second column, considered to estimate parameters θ_r, α, n and m, SimB: results of the third column, considered to estimate parameters θ_s, θ_r, α, n and m, PTF1: without the input of the $\theta(h)$ point and PTF2: with the input of the $\theta(h)$ point.

The parameters α and n are empirical constants related with the shape and curvature of the SWRC (van Genuchten and Nielsen, 1985, van Genuchten et al. 1991). Their estimates were inaccurate (Table 2) in most scenarios, showing that they were sensitive to the non-linear fitting procedure, also reported by Wösten et al. (2001), Pachepsky and Rawls (2004) and Silva et al. (2017a). However, estimates of the parameter n with the Splintex 2.0-PTF2-simB were strongly correlated (r = 0.704) to "measured" data whereas a weak correlation was found (r = 0.052) using Splintex 1.0-PTF2 for the sandy texture. Regarding the clayey texture, the r values yielded with the Splintex 2.0 estimates ranged from –0.253 to 0.45, against –0.363 to 0.314 obtained using Splintex 1.0.

The values of α obtained from those PTFs were dispersed, compared to this parameter fitted with measured data, showing in some cases negative correlations for both Splintex versions. However, a small improvement in the estimation of α was noticed with Splintex 2.0-PTF1-simB in comparison with Splintex 1.0-PTF1. The values of r for loamy and silty loam texture varied from –0.123 to 0.017 and from 0.139 to 0.156, respectively. Overall, the correlation of α estimated with Splintex 1.0- PTF2 ranged between –0.147 and 0.535 whereas with Splintex 2.0-PTF2-simA between –0.149 and 0.248. Although some values of r for α estimates were not satisfactory, $\theta(h)$ is calculated by combining all parameters of equation 1 and not only α. Wösten et al. (2001) and Pachepsky and Rawls (2004) in their review about PTFs, where different types of soils and situations worldwide were considered, showed that estimates of α and n are often imprecise. Tomasella et al. (2000), Barros et al. (2013), Medeiros et al. (2014) and Reis et al. (2018) report similar understanding about these parameters and enhanced their marked variability in the evaluated soils.

2.5.3 The performance of Splintex 1.0 *versus* Splintex 2.0 for the SWRC' estimation

The output options of both versions of Splintex were compared describing simulation A (where three parameters were estimated) and simulation B (where four parameters were estimated).

The difference between values of RMSE, EMA and r (Table 3) for Splintex 1.0-PTF1 *versus* Splintex 2.0-PTF1-simA and -simB and for Splintex 1.0-PTF2 *versus* Splintex 2.0-PTF2-simA and -simB was significant. However, a small improvement was observed when the estimation of Splintex 2.0-PTF2-simB and Splintex 1.0-PTF2 were compared, since RMSE reduced from 0.08 to 0.06 m^3 m^{-3} and MAE from 0.06 to 0.03 m^3 m^{-3} for clayey and sandy textures. Except for the sandy and sandy loam textures, both precision and accuracy of the parameters estimation diminished (Table 3). Splintex 2.0-PTF2-simB showed high correlation for all textures, yielding r values that ranged from 0.83 to 0.92. Although the estimates of the parameters θ_r, α and n showed low precision, the estimated SWRCs were close with ones yielded with the measured data.

Table 3: Statistical metrics of precision and accuracy to describe the performance of Splintex 1.0 and 2.0 to estimate water retention data.

Statistic	Splintex 1.0 PTF1	Splintex 1.0 PTF2	Splintex 2.0-PTF1		Splintex 2.0-PTF2	
			simA	simB	simA	simB
	Clayey					
RMSE	0.104	0.080	0.100	0.101	0.073	0.063
MAE	0.082	0.065	0.080	0.080	0.059	0.051
r	0.700	0.836	0.727	0.736	0.789	0.840
	Silty clay					
RMSE	0.105	0.080	0.111	0.112	0.092	0.115
MAE	0.090	0.068	0.095	0.096	0.074	0.097
r	0.749	0.824	0.771	0.784	0.788	0.862
	Sandy clay					
RMSE	0.083	0.071	0.084	0.089	0.076	0.057
MAE	0.067	0.058	0.069	0.073	0.063	0.044
r	0.761	0.814	0.791	0.816	0.794	0.873
	Clay loam					
RMSE	0.096	0.091	0.096	0.110	0.095	0.092
MAE	0.082	0.078	0.081	0.088	0.082	0.077
r	0.808	0.829	0.816	0.815	0.808	0.833
	Silty loam					
RMSE	0.132	0.136	0.145	0.155	0.141	0.156
MAE	0.095	0.097	0.104	0.108	0.098	0.109
r	0.826	0.819	0.822	0.853	0.829	0.862
	Loamy					
RMSE	0.108	0.101	0.114	0.122	0.097	0.101
MAE	0.086	0.079	0.090	0.096	0.076	0.077
r	0.878	0.884	0.892	0.905	0.914	0.906
	Sandy loam					
RMSE	0.354	0.179	0.093	0.098	0.082	0.075
MAE	0.097	0.073	0.077	0.082	0.068	0.063
r	0.363	0.684	0.806	0.827	0.848	0.866
	Sandy					
RMSE	0.840	0.077	0.097	0.093	0.077	0.057
MAE	0.170	0.061	0.074	0.074	0.056	0.035
r	0.220	0.869	0.804	0.843	0.911	0.918
	Sandy clay loamy					
RMSE	0.114	0.119	0.094	0.097	0.072	0.064
MAE	0.082	0.058	0.078	0.082	0.056	0.052
r	0.663	0.714	0.773	0.827	0.825	0.826

RMSE: root mean square error, MAE: mean absolute error, r: coefficient of Pearson correlation, SimA: results of the second column, considered to estimate parameters θ_r, α, n and m, SimB: results of the third column, considered to estimate parameters θ_s, θ_r, α, n and m, PTF1: without the input of the $\theta(h)$ point and PTF2: with the input of the $\theta(h)$ point.

These results indicate that the estimation of SWRC by Splintex 2.0 may contribute to the indirect quantification of key-soil-hydraulic variables. PTFs contribute to water balance simulations and had their importance in hydrological and agricultural models highlighted by De Jong van Lier et al. (2015), who estimated the plant available water capacity for several Brazilian and international soils.

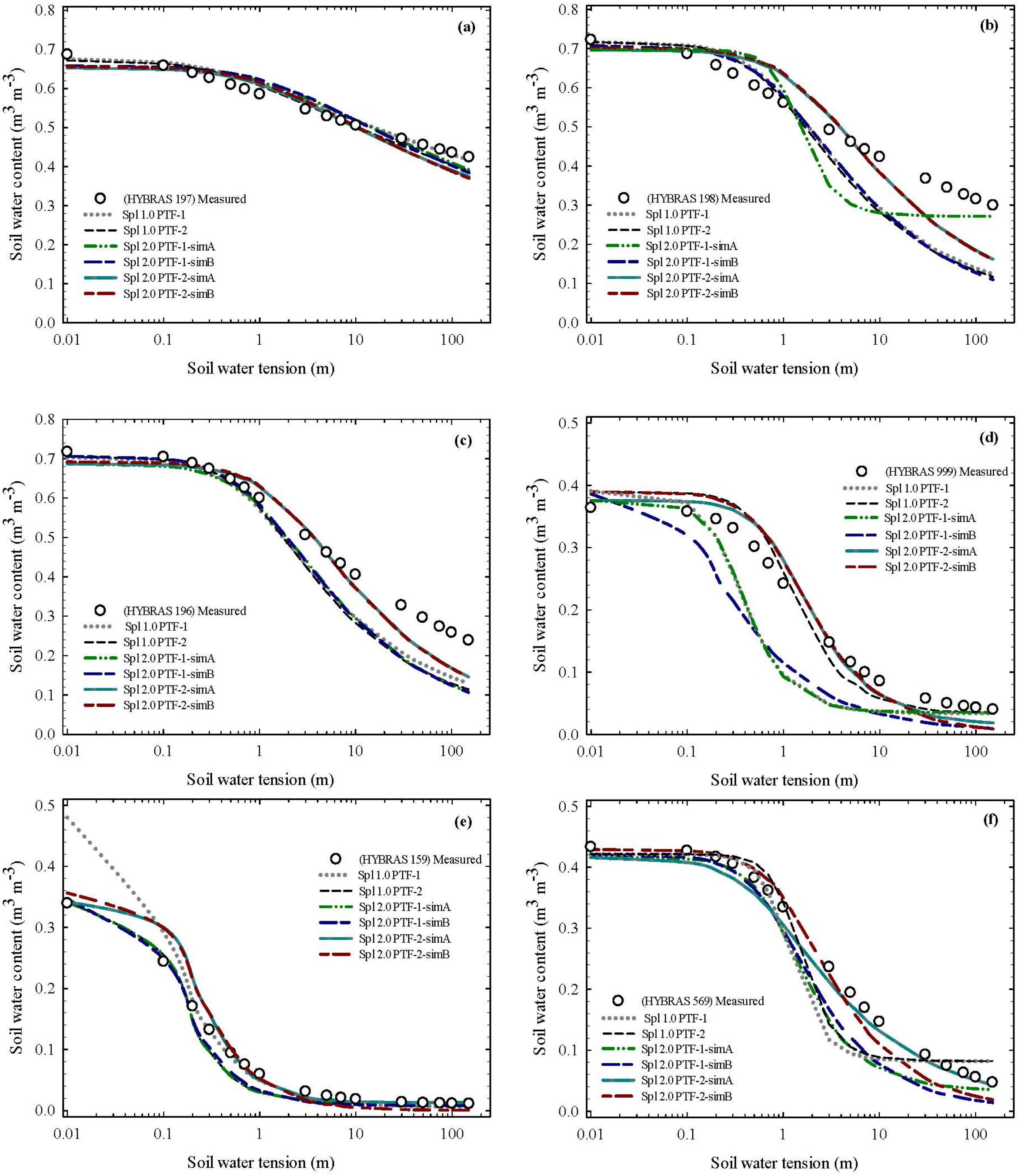

Figure 3 - Some examples of measured SWRCs and estimated curves with Splintex 1.0-PTF1, Splintex 1.0-PTF2, Splintex 2.0-PTF1-simA and simB, Splintex 2.0-PTF2-simA and simB for six main groups of soil texture available in HYBRAS database. (a) Clayey, (b) Clayey loam, (c) Silty clay loam, (d) Sandy loam, (e) Sandy and (f) Loamy.

The performance of both Splintex versions can be visually compared against measured SWRCs for six main texture groups (Figures 3a-f). In general, Splintex-PTF2-simA and

Splintex-PTF2-simuB estimated the closest SWRCs to the measured data. This small improvement may be linked to the input of the measured water content *θ(1.0 m)* of the evaluated soils that enhanced the *θ(h)* estimates and should therefore be preferred whenever possible., The results of θ yielded with Splintex were overestimated for h values between 0.10 and 1.0 m (Figure 3b) and underestimated for h values larger than 1.0 m (Figure 3c). In contrast, for small values of h, both models showed the same behavior, except for the sandy textured soil (Figure 3e) that had θ near saturation overestimated with Splintex 1.0-PTF1. The results obtained with Splintex showed that the input variables ρ_b, ρ_p, θ_s (or ϕ) and a $\theta(h)$ point were necessary for a better SWRC estimation.

2.5.4 The performance of Splintex 2.0 in the estimation of the hydraulic conductivity curve

The measures of performance of Splintex 2.0 to estimate the function $K(\theta)$ are presented in table 4 and figure 4. The statistical indices showed mean values of the parameters θ_s and m close to the same regressed with measured data. The same result was not identified for parameters λ and K_s. However, a strong correlation (r = 0.80) was found when $K(\theta)$ was analyzed on logarithmic scale, revealing a RMSE of 0.89.

The correlation matrix of the $K(\theta)$ parameters estimated with Splintex 2.0 (Table 4) revealed moderate correlation (r = 0.663, P-value=0.15) between parameters λ and m, strong and significant correlation between parameters λ and θ_r (r = 0.988, P-value=0.0002) and weak correlation between θ_r and θ_s (r = -0.244, P-value=0.70). Similar results were observed by Weynants et al. (2009), who developed new PTFs based on equations 1, 2 and 3 using data from Vereecken (1988).

Table 4: Fitted and estimated VGM parameters of the hydraulic conductivity curve and their matrix of correlation for six UNSODA data set.

UNSODA Code	θ_s ($m^3 m^{-3}$)	θ_r ($m^3 m^{-3}$)	m	λ	$\log_{10}[K_s$ (cm d^{-1})]	r	RMSE

	Fitted parameters						
1050_ *Sandy*	0.391	0.097	0.990	2.331	1.80	0.971	2.018
1051_ *Loamy s.*	0.406	0.010	0.807	1.847	2.30	0.967	0.823
1063_ *Sandy*	0.428	0.058	0.990	1.167	2.82	0.972	0.786
1130_ *Sandy l.*	0.373	0.257	0.663	0.498	1.22	0.956	0.333
3130_ *Loamy s.*	0.669	0.197	0.990	0.140	2.03	0.939	0.614
3160_ *Loamy s.*	0.508	0.145	0.990	1.657	2.29	0.987	1.106
Mean	0.463	0.128	0.905	1.273	2.08	0.965	0.947
	Estimated parameters with Splintex 2.0						
1050_*Sandy*	0.406	0.003	0.761	0.506	1.63	0.983	1.190
1051_*Loamy s.*	0.410	0.023	0.949	1.494	1.67	0.971	0.749
1063_*Sandy*	0.425	0.002	0.761	0.503	1.68	0.976	0.787
1130_*Sandy l.*	0.410	0.005	0.569	0.526	1.67	0.985	1.515
3130_*Loamy s.*	0.581	0.005	0.435	0.537	1.73	0.973	0.759
3160_*Loamy s.*	0.448	0.006	0.403	0.547	1.87	0.957	0.576
Mean	0.447	0.007	0.646	0.686	1.71	0.974	0.929
Splintex 2.0	Correlation matrix with fitted parameters						
θ_s (m^3 m^{-3})	1	-	-	-	-	-	-
θ_r (m^3 m^{-3})	-0.202	1	-	-	-	-	-
m.	-0.612	0.549	1	-	-	-	-
λ	-0.244	0.988*	0.663	1	-	-	-
log$_{10}$[K_s (cm d^{-1})]	0.355	-0.047	-0.709	-0.174	1	-	-

Loamy s.: Loamy sand, Sandy l.: Sandy loam, RMSE: root mean square error, *r*: coefficient of Pearson correlation, θ_s: saturated water content, θ_r: residual water content, λ and *m*: 1-1/*n*, K_s: fitted matching point at saturation, *: significant at *P*-value=0.02% and other correlation values were not because their *P*-values were larger than 5%.

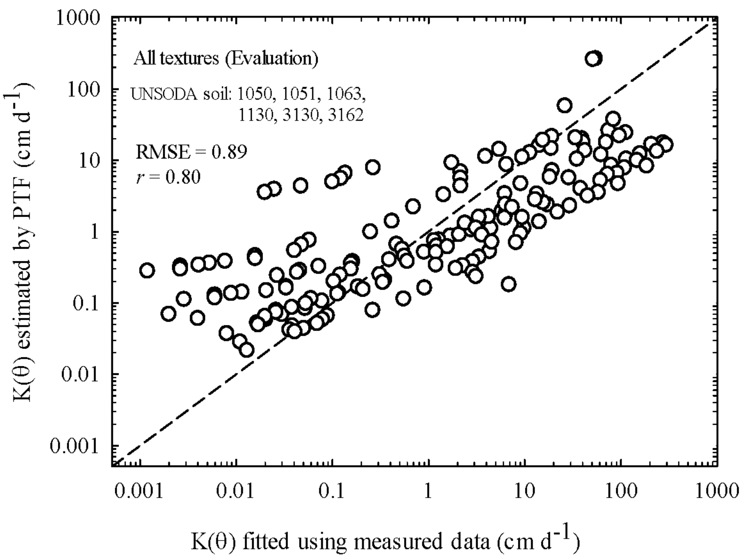

Figure 4 - Estimation of *K(θ)* fitted with measured data plotted against *K(θ)* estimated with Splintex 2.0 for six UNSODA data set.

The function *K(θ)* fitted with measured data and estimated with Splintex 2.0 are presented in figure 5 and table 4. Although the *K(θ)* values were not well estimated for the dry range of the SHCC, they were well estimated at the near saturation range (Figure 5a), (UNSODA 1050 and 1130). However, for some other points (UNSODA 1063 and 3130), the *K(θ)* estimates matched with some fitted values using measured data at the dry range (Figure 5b) and presented better performance in representing the SHCCs of UNSODA 1051 and 3160 all over the curve ranges (Figure 5c).

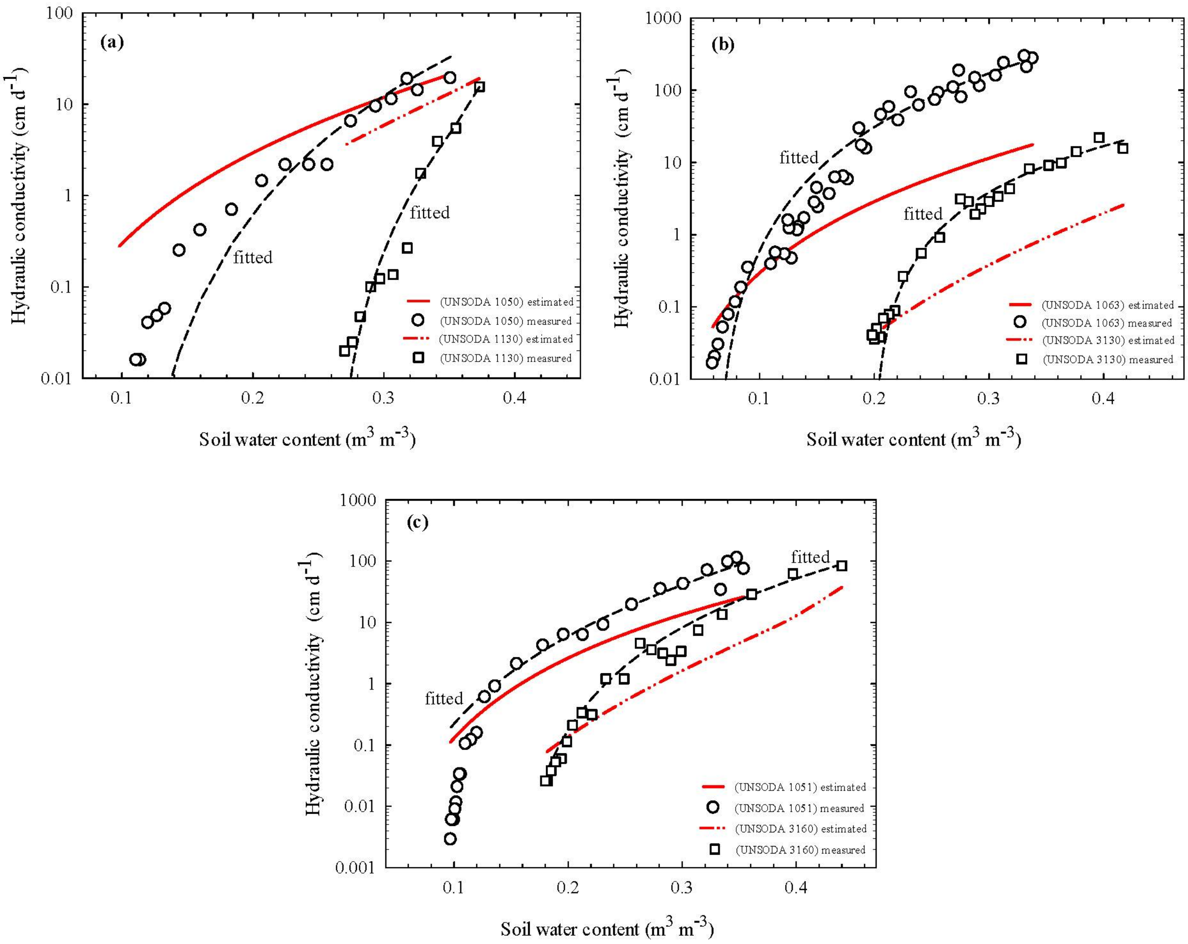

Figure 5 - Comparison between estimated and fitted SHCC using measured data: (a) best Splintex estimation for the wet range of *K(θ)*, (b) best Splintex estimation for the dry range of *K(θ)* and (c) best Splintex estimation for the entire curve of *K(θ)*.

Two reasons may explain why *K(θ)* values were not well estimated for any curve. First, it is well known that *K(θ)* is affected by the tortuosity and continuity of the pores, which are not directly related to the soil texture (Weynants et al., 2009). Second, measuring *K(θ)* is difficult due to the high variation present in the experimental soil samples and the long time needed to reach the equilibrium at each *h* value imposed (Karup et al., 2017). Furthermore, variations in experimental procedures and associated errors may introduce additional noise into experimental data (Zhang and Schaap, 2019; Ottoni et al., 2019). Therefore, the predictors used in Splintex 2.0 were not sufficient to estimate *K(θ)* evidencing that this estimation procedure claims for other measurable physical characteristics of soils that have influence on the structure of pores. Nevertheless, these characteristics should be easily measured because the main aim of a PTF is to be benefited from easy-obtained soil properties. One interesting addition variable might be a measured *K(θ)* point-value, as done in the estimation of the SWRC parameters.

2.6 CONCLUSIONS

A new PTF model (Splintex 2.0) was presented in this study, which was programmed in C++ language with a user-friendly interface and that can be applied to any porous medium, without the calibration need, for estimating the parameters of the VGM equations for SWRC and SHCC. The Splintex 2.0 algorithm was written to convert PSD and mass fractions into pore size distribution as accomplished in the previous version. This model provides two-main PTF options for estimating SWRC, allowing users to decide about using θ_s as a statistical-fitting parameter or to the measured total porosity. The SWRC parameters were better estimated with Splintex 2.0 than with Splintex 1.0, where the functions Splintex 2.0-PTF2-simA and Splintex 2.0-PTF2-simB performed better for the textures analyzed, decreasing the bias of the model. Furthermore, Splintex 2.0 estimated the SHCC parameters assuming that soil pores can be represented by equivalent capillary tubes and that the water flow can be plotted knowing the pore size distribution. This approach was not present in its previous version, which was built in BASIC language to run only one SWRC per time and to print the estimates on the computer window. Splintex 2.0 runs simultaneously several SWRCs and SHHCs exporting all results in a *.txt* file, emphasizing the model improvement. The estimates of K_s with Splintex 2.0 were closer to the measured K_s. For some soils (UNSODA 1051 and 3160), the new computer model estimated the complete SHCC with slight underestimation, requiring further-additional input variables to improve the estimation of *K(θ)*.

2.7 REFERENCES

Arruda, F.B., Zullo, J.J., Oliveira, J.B., 1987. Soil parameters for the calculation of the available water based on soil texture. **Revista Brasileira de Ciência do Solo**. 11, 11–15.

Arya, L.M., Paris, J.F., 1981. A physico-empirical model to predict the soil moisture characteristic from particle-size distribution and bulk density data. **Soil Science Society of America Journal**. 45, 1023–1030.

Arya, L.M., Richeter, J.C., Davidson, S.A., 1982. A comparison of soil moisture characteristic predicted by the Arya-Paris model with laboratory-measured data. **Agristars Technology Resport**. Sm-L1-04247, JSC-17820, NASA-Johson Space Center, Houston, TX.

Arya, L.M., Leij, F.J., Van Genuchten, M.Th., Shouse, P.J., 1999a. Scaling Parameter to Predict the Soil Water Characteristic from Particle-Size Distribution Data. **Soil Science Society of America Journal**. 63, 510–519.

Arya, L.M., Leij, F.J., Shouse, P.J., Van Genuchten, M.Th., 1999b. Relationship between the Hydraulic Conductivity Function and the Particle-Size Distribution. **Soil Science Society of America Journal**. 63, 1063–1070.

Arya, L.M., Heitman, J.L., 2015. A Non-Empirical Method for Computing Pore Radii and Soil Water Characteristics from Particle-Size Distribution. **Soil Science Society of America Journal**. 79, 1537–1544.

Barros, A.H.C., Van Lier, Q.J., Maia, A.H.N., Scarpare, F.V., 2013. Pedotransfer functions to estimate water retention parameters of soils in northeastern Brazil. **Revista Brasileira de Ciência do Solo**. 37, 379–391.

Bouma J., 1989. Using soil survey data for quantitative land evaluation. **Advanced Soil Science**. 9, 177–213.

Botula, Y.D., Cornelis, W.M., Baert, G., Van Ranst, E., 2012. Evaluation of pedotransfer functions for predicting water retention of soils in the Lower Congo (D.R. Congo). **Agricultural Water Management**. 111, 1–10.

De Jong van Lier, Q., Wendroth, O., Van Dam, J., 2015. Prediction of winter wheat yield with the SWAP model using pedotransfer functions: An evaluation of sensitivity, parameterization and prediction accuracy. **Agricultural Water Management on Science Direct**. 154, 29–42.

Haghverdi, A., Öztürk, H.S., Cornelis, W.M., 2014. Revisiting the pseudo continuous pedotransfer function concept: Impact of data quality and data mining method. **Geoderma**. 227, 31–38.

Karup, D., Moldrup, P., Tuller, M., Arthur, E., Jonge, L.W., 2017. Prediction of the soil water retention curve for structured soil from saturation to oven-dryness. **European Journal of Soil Science**. 68, 57-65.

Nemes, A., Schaap, M.G., Leij, F.J., Wosten, J.H.M., 2001. Description of the unsaturated soil hydraulic database UNSOSA version 2.0. **Journal of Hydrology**. 251, 151–162.

Ottoni, M.V., Ottoni, F.T.B., Schaap, M.G., Lopes-Assad, M.L.R.C., Rotunno, F.O.C., 2018. Hydrophysical database for Brazilian soils (HYBRAS) and pedotransfer functions for water retention. **Vadose Zone Journal**. 17, 1–17.

Ottoni, M.V., Ottoni, T.B., Lopes-Assad, M.L.R.C., Rotunno, O.C., 2019. Pedotransfer functions for saturated hydraulic conductivity using a database with temperate and tropical climate soils. **Journal of Hydrology**. 575, 1345–1358.

Pachepsky, Y.A., Rawls, W.J., 2004. Development of Pedotransfer Functions in Soil Hydrology. In: Developments in Soil Science 30. **Elsevier**, Amsterdam. 525p.

Prevedello, C.L., Armindo, R.A. (Eds.), 2015. Física do solo: com problemas resolvidos. **2° Ed revisada e ampliada**. Celso Luiz Prevedello, Curitiba.

Prevedello, C.L., Loyola, J.M.T., 2002. Modelo para estimar as propriedades hidráulicas de meios porosos a partir da curva granulométrica. **Congresso Brasileiro de Mecânica dos Solos e Engenharia Geotécnica**, São Paulo, 2002. ABMS, Anais. São Paulo, pp. 467–472.

Prevedello, C.L., Maggiotto, S.R., Loyola, J.M.T., Dias, N.L., Bepler Neto, G. 2007. Water balance for automatic data acquisition in culture of wheat (Triticum aestivum L.). **Revista Brasileira de Ciência do Solo**. 31, 1–8.

Reis, A.M.H., Armindo, R.A., Duraes, M.F., Lier., Q.J.V., 2018. Evaluating pedotransfer functions of the Splintex model. **European Journal of Soil Science**. 69, 685–697.

Rodas, A., 1970. Determinación de la conductividad hidráulica em muestras de suelo inalterada. Lima, **CENDRET. 118p**.

Scussiato, T., 2012. Study of the air flow in soils using the technique of air sparging in bidimensional physical model. **MSc thesis, Universidade de São Paulo, Piracicaba**. URL http://www.teses.usp.br/teses/disponiveis/3/3145/tde-11062013105342/en.php [accessed on 05 January 2019].

Silva, A.C., Armindo, R.A., Brito, A.S., Schaap, M.G., 2017a. Splintex: A physically-based pedotransfer function for modeling soil hydraulic functions. **Soil Tillage Research**. 174, 261–272.

Silva, A.C., Armindo, R.A., Brito, A.S., Schaap, M.G., 2017b. An assessment of pedotransfer function performance for the estimation of spatial variability of key soil hydraulic properties. **Vadose Zone Journal**. 16, 1–10.

Souza, J.L.M., Gomes, S., 2008. Limitations in the use of a ten-day water balance model, based on available water capacity in the soil. **Acta Scientiarum Agronomy**. 30, 153–163.

Tomasella, J., Hodnett, M.G., Rossato., L., 2000. Pedotransfer functions for the estimation of soil water retention in Brazilian soils. **Soil Science Society of America Journal**. 64, 327–338.

Tomasella, J., Hodnett, M.G., Cuartas, L.A., Nobre, A.D., Waterloo, M.J., Oliveira, S.M., 2008. The water balance of an Amazonian micro-catchment: the effect of interannual variability of rainfall on hydrological behaviour. **Hydrological Processes**. 22, 2133–2147.

Van Genuchten, M.Th., 1980. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. **Soil Science Society of America Journal**. 44, 892–897.

Van Genuchten, M.Th., Nielsen, D.R., 1985. On describing and predicting the hydraulic properties. **Annales Geophysicae**. 3, 615–628.

Van Genuchten, M.Th., Leij, F.J., Yates, S.R., 1991. The RETC Code for Quantifying the Hydraulic Functions of Unsaturated Soils, Version 1.0. **EPA Report 600/2-91/065, U.S. Salinity Laboratory, USDA, ARS, Riverside**, California.

Vaz, C.M.P., Iossi, M.F., Naime, J.M., Macedo, A., Reichert, J.M., Reinert, D.J. et al. 2005. Validation of the Arya and Paris water retention model for Brazilian soils. **Soil Science Society of America Journal**. 69, 577–583.

Wösten, J.H.M., Pachepsky, Y.A., Rawls, W.J. 2001. Pedotransfer functions: bridging the gap between available basic soil data and missing soil hydraulic characteristics. **Journal of Hydrology**. 251, 123–150.

Zhang, Y., Schaap, M., 2017. Weighted recalibration of the Rosetta Pedotransfer model with improved estimates of hydraulic parameter distributions and summary statistics (Rosetta3). **Journal of Hydrology**. 547, 39–53.

Zhang, Y., Schaap, M., 2019. Estimation of saturated hydraulic conductivity with pedotransfer functions: A review. **Journal Hydrology**. 575, 1011–1030.

Vereecken, H. 1988. Pedotransfer functions for the generation of hydraulic properties for Belgian soils. **Ph.D. diss. Katholieke Universiteit Leuven**, Leuven, Belgium.

Vogel, H.J., Roth, K., 2003. Moving through scales of fl ow and transport in soil. **Journal Hydrology**. 272,95–106.

Weynants, M., Vereecken, H., Javaux, M., 2009. Revisiting Vereecken Pedotransfer Functions: Introducing a Closed-Form Hydraulic Model. **Vadose Zone Journal**. 8, 86–95.

3 CHAPTER II: SPLINTEX 2.0: IMPROVING A PHYSICO-EMPIRICAL MODEL FOR ESTIMATING PARAMETERS OF THE SOIL WATER RETENTION CURVE

3.1 ABSTRACT

Soil water retention governs how much water can be retained in soil and available for plants. Soil water retention curve (SWRC) plays an important role in the understanding and modeling soil hydraulic processes. However, measuring SWRC is an expensive procedure and as such unfeasible for large-scale monitoring. Indirect quantification is a rapid and low cost alternative to obtain SWRC. Some empirical pedotransfer functions (PTFs) have been published to estimate SWRC from particle size distribution (PSD) and other basic soil information. However, these PTFs are often calibrated with soil data from temperate climate-region, therefore their usage brings uncertainties to tropical soils. Splintex 2.0 was developed with a user-friendly computational interface for estimating parameters of soil hydraulic functions based on a physico-empirical model. Splintex 2.0 establishes the relationship between PSD and SWRC by converting soil solid mass fractions into water content and the distribution of porosity into pressure head. Splintex 2.0 computational procedures and equations were written in C++ language, and its estimation is improved when one or two measured points of the SWRC are added, without requiring any calibration data. This model was tested using a database of 1,355 samples from several countries, thus allowing a more detailed quantification of the univariate and bivariate probability distributions of the estimated parameters in different hydrogeology, climate and soil settings. The performance of the Splintex 2.0 model was evaluated by means of the linear correlation analysis (r) and systematic errors, using mean error (ME), mean absolute error (MAE), and root mean square error (RMSE). The Splintex 2.0 model performed well in the quantification of water retention with an RMSE = 0.082 $m^3 m^{-3}$ and r = 0.877. The goodness of fit of the Splintex 2.0 model was similar in comparison with other recognized PTF models. This model can be used universally for quantification SWRC for modelling purposes.

Keywords: Pedofunction. Pedotransfer function. Soil water release curve.

3.2 RESUMO

A retenção de água no solo determina a quantidade de água que pode estar retida no solo e disponível para as plantas. Uma função importante para o entendimento e modelagem de processos hidráulicos do solo é a curva de retenção de água (CRA). No entanto, sua medição completa é onerosa e, portanto, inviável para monitoramento em grande escala. Assim, alternativas de quantificação indireta que sejam rápidas e de baixo custo são alternativamente interessantes. Algumas funções de pedotransferência (FPTs) foram publicadas para estimar a CRA a partir da distribuição do tamanho de partículas (PSD) e outras informações físicas básicas do solo. No entanto, essas FPTs foram calibradas a partir de solos de regiões temperadas, o que significa que elas podem apresentar incertezas quando aplicadas em solos de regiões tropicais ou subtropicais. O Splintex 2.0 foi desenvolvido para estimar parâmetros de funções hidráulicas do solo com base em um modelo físico-empírico que pode ser aplicado universalmente. Splintex 2.0 é uma versão evoluída do Splintex 1.0, com todos os procedimentos computacionais e equações escritas em linguagem C++, estabelecendo a relação entre PSD e CRA a partir da conversão das frações de massa sólida em umidade e distribuição de poros em tensão de água no solo. O modelo Splintex foi testado utilizando um banco de dados de 1.355 amostras de vários países, permitindo assim a quantificação mais detalhada das distribuições de probabilidade univariada e bivariada dos parâmetros estimados em diferentes configurações de hidrogeologia, clima e solo. O desempenho do modelo Splintex 2.0 foi avaliado por meio de análise de correlação linear (r) e erros sistemáticos, utilizando o erro médio (EM), erro médio absoluto (EMA) e a raiz quadrada do erro médio (RMSE). O modelo Splintex 2.0 apresentou bom desempenho na quantificação da umidade, revelando RMSE = 0,082 m^3 m^{-3} e r = 0,877. A qualidade do ajuste do modelo Splintex 2.0 foi semelhante a de outros modelos de FPT reconhecidos internacionalmente.

Palavras-chave: Pedofunção. Função de pedotransferência. Curva característica da água no solo.

3.3 INTRODUCTION

The quantification of water dynamics in the vadose zone of the soil requires extensive knowledge of hydraulic properties and functions (Zhang et al., 2016; Silva et al., 2017a; Zhang and Schaap, 2017). However, the measurement of these functions, such as soil hydraulic conductivity curve (SHCC) and soil water retention curve (SWRC) are, in general, expensive tasks, since they depend on laboratory measurement with specialized equipment. In addition, a large number of samples is required to identify the natural spatial variability of soil properties, raising the cost of such analysis (Silva et al., 2017b).

There is a wide number of practical and scientific applications of SWRC, including determination of drainable porosity (Ribeiro et al., 2007), field capacity (Jong van Lier, 2017), available water (Silva et al., 2017a), horizontal and vertical infiltration (Prevedello and Armindo, 2016), and hydraulic conductivity (van Genuchten, 1980; Rudiyanto et al., 2015).

Pedotransfer functions (PTFs) have been proposed and utilized as a method for estimating soil properties and hydraulic functions, which can circumvent measurement difficulties, allowing soil data to be used in large-scale simulation (McBratney et al., 2002; van Looy et al., 2017). This term, first introduced by Bouma (1989), was defined as empirical functions to estimate water or other edaphic soil properties which are difficult to measure from more readily available data (e.g., texture, soil organic carbon and bulk density).

Researchers as Schaap et al. (2001), Minasny and McBratney (2002), Tomasella et al. (2000), Tomasella et al. (2008), Haghverdi et al. (2014), Jong van Lier et al. (2015), Zhang and Schaap (2017), Reis et al. (2018) and Chaney et al. (2019) have developed or used PTFs to estimate the parameters of the SWRC according to van Genuchten (1980)-Mualem (VGM) model using regression models that consider basic soil physical attributes as input variables.

Many PTFs were developed for soils of temperate regions in the USA and Europe. However, PTFs developed for tropical soils, specifically for Brazil, are still scarce (Medrado and Lima, 2014). An important deadlock in building PTFs to tropical soils is because they may yield large uncertainty due to the empiricism inherent in the data and statistical methods used. Furthermore, PTFs developed for a specific Brazilian region may be not necessarily applicable to other regions due to the enormous soil variation.

In Brazil, PTFs have been developed by various researchers, as Tomasella and Hodnett (1998), Oliveira et al. (2002), Prevedello and Loyola (2002), Reichert et al. (2009), Michelon et al. (2010) and Barros et al. (2013). These authors analyzed physical data of soils from the Amazon and Northeast regions as well as the states of Pernambuco and Rio Grande do Sul for estimating parameters or water content at specific points of the SWRC. Tomasella et al. (2000)

and Hodnett and Tomasella (2002) suggested that their studies are applicable at the regional scale, since they used information from more than 500 soil horizons from different regions.

The development of PTFs based on physical principles is an alternative to overcome the empiricism inherent to estimate water or other edaphic soil properties using regression analysis or pure physic-mathematical models. Prevedello and Loyola (2002) developed a computer program, the Splintex 1.0 (Silva et al., 2017a; Silva et al., 2017b; Reis et al., 2018), using BASIC language, built to estimate the parameters of the VGM equation based on a physico-empirical approach. This computer model uses a simplification of the approach by Arya and Paris (1981), hereafter referred to as the AP model, for translating PSD data into a solid mass fraction and then into soil water content (θ), as well as the distribution of porosity into soil water tension (h). Splintex 1.0 estimation can be improved when one or two measured points of the SWRC (Reis et al., 2018) are included in the calculation. Because Splintex 1.0 is based on the capillarity principle, this model can be applied to any porous medium without needing model calibration (Silva et al., 2017a; Reis et al., 2018).

The performance of Splintex 1.0 was evaluated by Silva et al. (2017a) based on 103 sample points from Brazil, and Silva et al. (2017b) using 60 points from a sandy area to simulate the spatial variation of soil hydraulic properties. Reis et al. (2018) also tested its performance by comparing the effect of the input of a measured point of the SWRC for 50 sample points.

The aim in this study is to present a new-developed version of the Splintex model (Splintex 2.0), written in C++ language, with a user-friendly interface. The model is then validated with two large databases from different regions of the world. Moreover, the results were contrasted to two known-worldwide PTFs together with their sensitivity analysis for estimating field capacity.

3.4 MATERIAL AND METHODS

3.4.1 Data set and soil hydraulic parameters

The data set used in this study is a compilation from sources of data worldwide, including Australian data set (Minasny et al., 1999), Hydrophysical Database for Brazilian Soils - HYBRAS (Ottoni et al., 2018), Grenoble Catalogue of Soils - GRIZZLY (Haverkamp et al., 1997) and Unsaturated Soil Hydraulic Database - UNSODA (Nemes et al., 2001). The combined data set contains 1,130 samples of water retention curves with a total of 22,600 $\theta(h)$ points together with their basic soil properties. This large data set presented a wide variety of textural distribution for several countries (Figure 1) and were divided into the Brazilian and international databases.

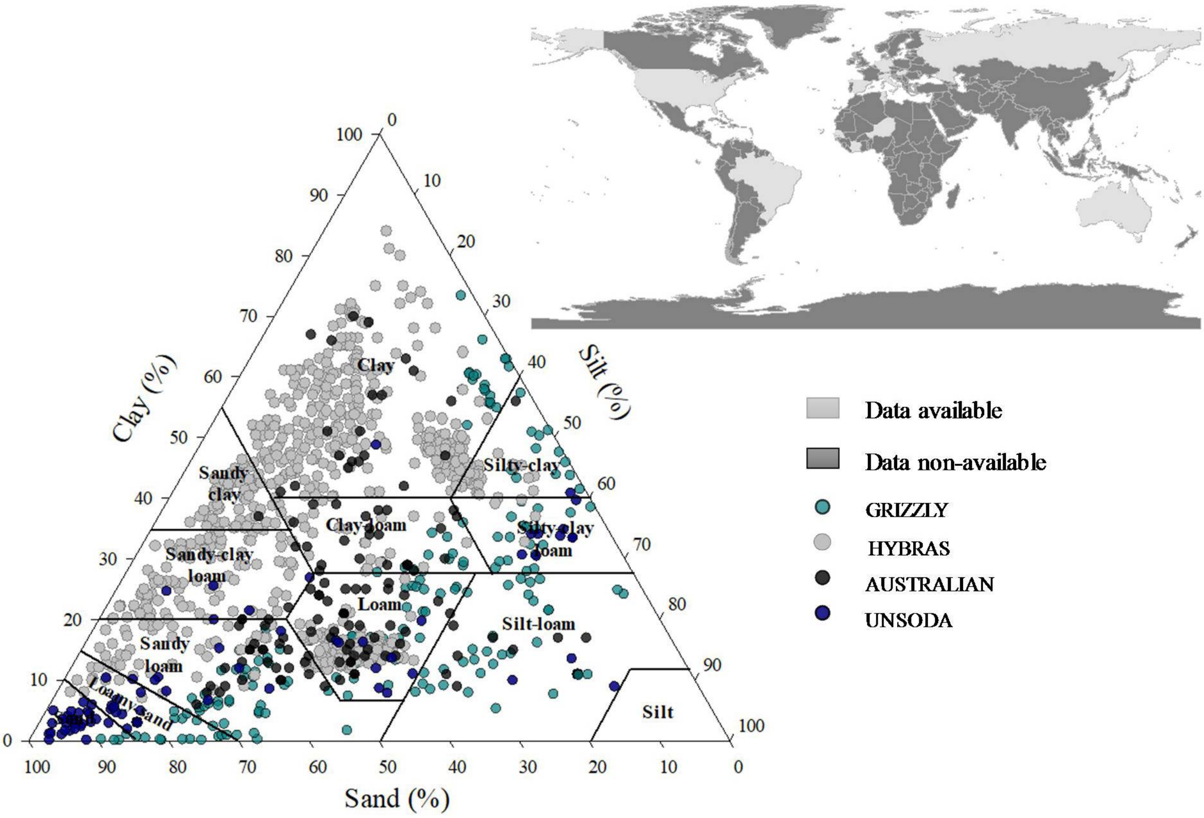

Figure 1 - Distribution of the 1,130 data sets along the USDA textural triangle (Soil Survey Staff, 1999) used to estimate the VGM parameters.

The soil water retention data were fitted to the VGM equation:

$$\theta(h) = \theta_r + (\theta_s - \theta_r) / \left[1 + (\alpha \cdot h)^n \right]^m \tag{1}$$

in which θ is the volumetric soil water content (m^3 m^{-3}) as a function of the soil water tension (h), with $h > 0$ for unsaturated conditions (m), θ_r and θ_s are respectively the residual and saturated water content (m^3 m^{-3}), α (m^{-1}) and n and m [m=1-1/n, parametric restriction of Mualem (1976)] are empirical curve shape parameters. In this study, h is defined as the modulus of the matric potential and expressed in units of energy per weight (m=J/N).

The parameters θ_s, θ_r, α, n and m were fitted for all data set using the non-linear optimization procedure, by using the 'nls' function available in software R (Armindo and

Wendroth, 2016; Zhang and Schaap, 2017). This technique is commonly applied to optimize the parameters of equation 1 for each soil sample by minimizing:

$$\sigma^2(p) = \sum_{i=1}^{N_w} \left[\theta_i - \theta_i'(h_i) \right]^2 \qquad (2)$$

in which σ^2 is the variance of each term in the squared distribution, θ_i and $\theta_i'(h_i)$ are measured and estimated water content of the i-th water retention data, respectively, p is the VGM parameter vector (θ_s, θ_r, α, n and m), which is used for estimating $\theta_i'(h_i)$ using corresponding h_i and N_w is the number of measured water retention data for each soil sample.

3.4.2 Splintex 2.0

The model Splintex 2.0 was developed based on its previous algorithm (Splintex 1.0), which was written in BASIC language by Prevedello and Loyola (2002) and described by Silva et al. (2017a) and Reis et al. (2018). The flowchart of Splintex 2.0 is presented in figure 2 indicating input and output data as well as the model interactions.

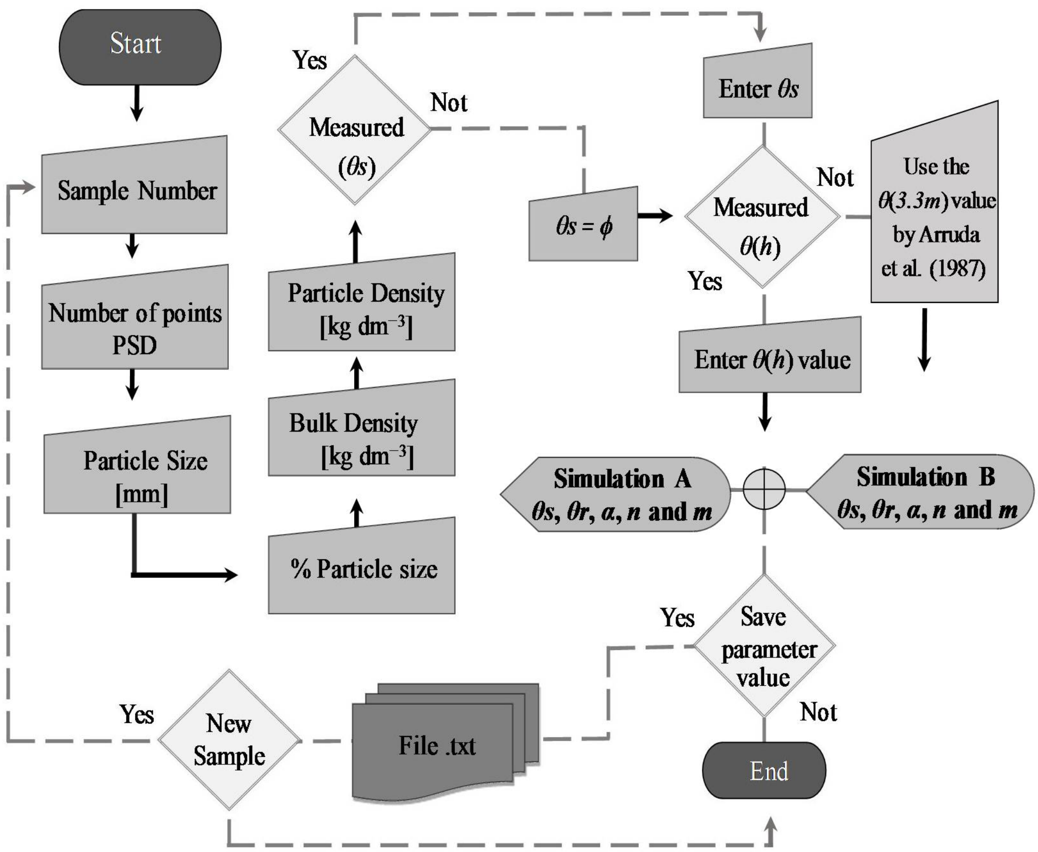

Figure 2 - Flowchart of the Splintex 2.0 algorithm. The output of the VGM parameters are presented in two ways; simulation A: θ_s was set as its measured value and θ_r, α, n and m estimated; simulation B: all parameters θ_s, θ_r, α, n and m estimated; PSD: particle size distribution.

Splintex 2.0 consists of a computer algorithm developed in C ++, compiled in an Integrated Programming Environment (IPE) CodeBlocks, structured with data input, mathematical interactions and data output. Splintex 2.0 presents some optional functions for estimating VGM parameters according to the availability of input data, and the user's decision of assuming θ_s as the only fitting parameter, or as an independent parameter (van Genuchten, 1980) with its physical meaning associated with total porosity. We assessed the performance of these functional options available in Splintex 2.0.

The Splintex 2.0 algorithm is based on the set of equations of the AP model for estimating the values of $\theta(h)$ with additional improvements. In the AP model, h is related to the pore radius (R_i) of the largest water-filled pore according to the Young–Laplace equation:

$$h_i \approx 2\sigma \cos(\omega) \big/ \rho_w \vec{g}\ R_i \tag{3}$$

in which h is the capillary rise (m), σ is the coefficient of surface tension at the air–water interface (kg s^{-2}), R_i is the radius of the largest water-filled pore (m), ω is the contact angle in the largest water-filled pore (AP model considers ω=0), ρ_w is the density of water (kg dm^{-3}) and g is the acceleration of gravity (m s^{-2}).

The values of θ are obtained from successive sum of water-filled pore volumes, according to the next equation:

$$\theta_i = \phi S_w \sum_{j=0}^{j=i} w_j;\ \ i = 1, 2, ..., n \tag{4}$$

in which ϕ is the total porosity of the sample (m^3 m^{-3}), S_w is the ratio of measured saturated water content to theoretical porosity and w_i is the solid mass of the i-th fraction (kg kg^{-1}).

The total effective volume of pores is distributed in the same proportion as the solid mass (Arya et al., 2015). Starting with the first fraction, calculated pore volumes are progressively added and considered to be filled with water. The value R_i is derived in equation 3 from the particle radius and together with a scale factor (β) for correcting the possible non-sphericity. The constant value of β = 1.38 suggested by AP worked well for some soils, but not for all particle size distributions. Arya et al. (1982) analyzed 181 soil samples from New Jersey and found values of $1.26 \leq \beta \leq 2.10$. Vaz et al. (2005) found an average value of β = 0.977 for 104 soil samples obtained from the South and Southeast regions of Brazil.

For Splintex 1.0, Prevedello and Loyola (2002) used 1.20 as an initial value of β. Unless the volumetric fraction of solid particles is smaller than 7.6% and the sum of the percentage of particles to the diameter 0.1 mm is smaller than 60%, β is then assumed to be 1.15. If the sum of the percentage of particles up to the diameter 0.1 mm is larger than 60%, β is set to 1.0. For other proportions, β is calculated according to Arya et al. (1999a) using:

$$\beta = \log_{10} N_i / \log_{10}(\tau_i) \tag{5}$$

in which N_i is the number of hypothetical spherical particles and τ_i the natural number of particles in the sample, respectively. A more complete description to obtain equation 5 is given in Arya and Paris (1999a).

The same procedure for β remained on the Splintex 2.0 because it yielded good fit performance for different soil samples. However, some deviations may occur in this procedure since the aim is to get the size and distribution of pores for deriving the SWRC, not the size and distribution of particles. These deviations can be eliminated if the user provides one (θ_s) or two experimental points of the retention curve. Otherwise, an automatic correction is accomplished based on the PTF of Arruda et al. (1987) estimating $\theta(3.3\ m)$ as follows:

$$\theta(3.3m) = 7.00138\rho_b \exp\left[3.9\times10^{-2}(\%Clay+\%Silt) - 2.6\times10^{-4}(\%Clay+\%Silt)^2\right] \tag{6}$$

in which $\theta(3.3\ m)$ is the soil water content ($m^3\ m^{-3}$) at the water tension h of 3.3 m and ρ_b is the bulk density (kg dm^{-3}).

The estimate described in equation 6 is used to find the best value of β. As β is estimated, h is calculated from equation 3 and θ_i from equation 4 for sixteen classes of particle diameters. The estimated $\theta(h)$ values were fitted to equation 1. In simulation A (Figure 2), only parameters θ_r, α and n were estimated with a fixed value of θ_s, whereas in simulation B (Figure 2), all parameters (θ_s, θ_r, α and n) were estimated.

As shown in figure 2, the Splintex 2.0 model is built with input and output data, as well as optional information provided by the user. First, this model requires the number of texture points to create a vector of dimension "*N*" continuously stored in its memory. PSD and the percentage equivalent to each fraction are then inserted. After inserting the values, a cubic spline function is fitted to data for determining the cumulative PSD. This step consists of a standardized 16 classes of particle diameters: 2, 4, 6, 8, 10, 20, 40, 50, 60, 80, 100, 200, 400, 600, 800 and 1000 μm. Splintex 2.0 also requires inputs of bulk density (ρ_b), particle density

(ρ_p) and, optionally, measured saturated soil water content (θ_s). If the value of θ_s is unknown, then it is considered equal to the total porosity $\phi = 1 - \rho_b/\rho_p$.

3.4.3 Comparing the performance of Splintex 2.0 with other PTFs

The performance of Splintex 2.0 for estimating SWRC parameters was compared to Splintex 1.0, and to two other widely known PTFs: Neuropack (Minasny and McBratney, 2002; Chaney et al., 2019) and Rosetta (Zhang and Schaap, 2017). Both PTFs are neural-network-based models and were calibrated with data from various countries around the world, thus yielding good performance in comparison with other published PTFs in the literature (Zhang and Schaap, 2017). Neuropack and Rosetta were calibrated with part of the international databased used in this study (i.e., UNSODA for both Neuropack and Rosetta, and GRIZZLY for Neuropack). Neuropack required inputs of *sand*, *clay*, ρ_b and θ_s while Rosetta uses *sand*, *silt*, *clay* and ρ_b. Rosetta also has other options of data input to provide better estimates but it requires inputs $\theta(3.3\ m)$ and $\theta(150\ m)$, making it difficult to compare in this study.

The performance of the soil water content at field capacity (θ_{fc}) obtained with the parameters of equation 1 estimated with these PTFs was also evaluated. In this study, θ_{fc} was assumed as $\theta(3.3\ m)$ (Richards and Weaver, 1944) based on a static criterion that selects θ for a specific value of h. More details about several methods to calculate field capacity by static and dynamic criteria and their implications on crop yield can be found in Armindo and Wendroth (2016) and Turek et al. (2018). However, this study is focused on only evaluating the performance of those PTFs to estimate a functional soil property, θ_{fc}.

3.4.4 Performance evaluation criteria

Measured and estimated hydraulic properties with the PTFs, as well as the physical soil attributes, were described with the following summary statistics: minimum, maximum, mean, standard deviation and coefficient of variation. As in other studies with PTFs (Zhang and Schaap, 2017; Reis et al., 2018), the goodness of fit was assessed with the Pearson correlation coefficient (r), mean error (ME), mean absolute error (MAE), and root mean square error (RMSE), as follows:

$$ME = \frac{1}{N}\sum_{i=1}^{n}\left(\theta_{est} - \theta_{mea}\right) \tag{7}$$

$$MAE = \frac{1}{N}\sum_{i=1}^{n}\left|\theta_{est} - \theta_{mea}\right| \tag{8}$$

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{n}\left(\theta_{est} - \theta_{mea}\right)^{2}} \tag{9}$$

in which θ_{mea} is the i-th measured variable, θ_{est} is the i-th estimated variable and N is the number data.

3.5 RESULTS AND DISCUSSION

3.5.1 Summary statistics of data sets used in this study

Descriptive statistics of the soil physical properties used in this study is presented in Table 1. The particle size in the Brazilian and international data sets are quite diverse from low sand content to high clay content. The mean value of clay content is higher in the Brazilian database than in the international one. This is due to the dominant tropical soils in the database presenting conditions of high temperature and precipitation when associated with good drainage, favour weathering and, consequently, the formation of soils with an accumulation of minerals of 1:1 clay and Fe and Al oxides.

Table 1: Ranges of soil texture (according to USDA classification), bulk density (ρ_b), particle density (ρ_p) and total porosity (ϕ) for the assessed Brazilian and international soils.

Summary	Fractions (% mass)			ρ_p	ρ_b	ϕ
	Sand	Silt	Clay	kg dm^{-3}		%
	Brazilian database					
Maximum	90.0	54.4	84.0	2.970	1.710	68.6
Mean	41.7	22.4	35.9	2.602	1.408	45.7
Minimum	6.00	2.00	7.05	2.400	0.767	30.10
SD	18.7	13.6	17.7	0.102	0.204	8.65
CV (%)	44.7	60.8	49.2	3.90	14.5	18.9
	International database					
Maximum	97.5	79.0	73.4	2.820	1.810	66.8
Mean	44.0	34.3	21.8	2.644	1.504	42.9
Minimum	0.35	1.00	0.15	2.380	0.860	20.0
SD	26.5	16.7	16.9	0.06	0.148	6.75
CV (%)	60.2	48.7	77.9	2.45	9.82	15.8

SD: standard deviation and CV: coefficient of variation.

3.5.2 The Splintex 2.0 model

Splintex 2.0 provides an interface (Figure 3) wherein the user can manually enter or import values of input variables to estimate parameters of equation 1.

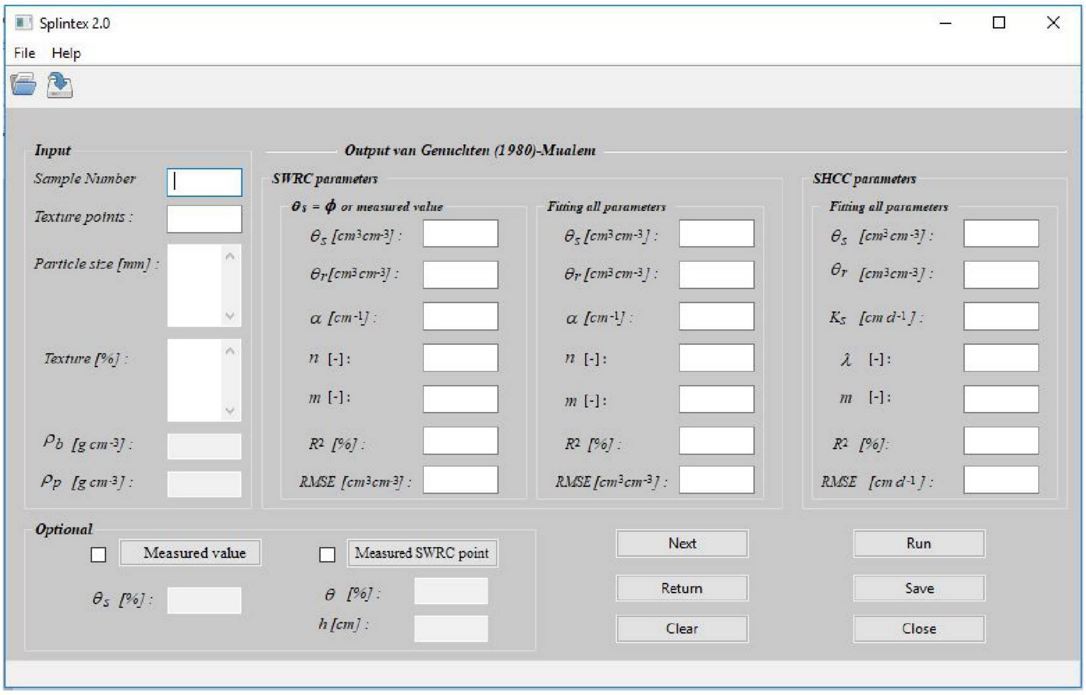

Figure 3 - Display window of Splintex 2.0 with data input and output of the results.

The Splintex 2.0 user interface (Figure 3) contains input and output boxes.

The required inputs are:

In the first column, it is necessary to insert sequentially the value of the sample number, number and diameter (mm) of the particle size distributions respectively, texture distribution (%), ρ_b (g cm^{-3}), ρ_p (g cm^{-3}), and the optional measures of θ_s and other $\theta(h)$ point of the SWRC.

The output is divided in:

- Two ways of outputs of the parameters of equation 1 are presented. The second column is simulation A, where four parameters (θ_r, α, n and m) are estimated and θ_s is considered as a measured value or equal to total porosity. Simulation B is in the third column where all five parameters (θ_s, θ_r, α, n and m) are estimated.

- The fourth column provides estimates of parameters of the unsaturated hydraulic conductivity $K(\theta)$. The estimation of $K(\theta)$ parameters is performed based on the model of Arya et al. (1999b) and Arya et al. (2015). And as results are presented the values of the parameters θ_s, θ_r, K_s, λ and m of the VGM. However, this study does not deal with the estimation of hydraulic conductivity.

3.5.3 The performance of Splintex 2.0 against three PTFs

The accuracy of several PTFs in estimating SWRC was evaluated dividing data into two sets: a Brazilian and an international database. It is not our intention to point out that an individual PTF should be applied only to soils from a specific country, but only to evaluate the performance of PTFs that were not calibrated with data set from Brazil. The following PTFs were compared:

- PTF2 of Splintex 1.0 is a physical-empirical PTF that can be applied to any porous medium without needing calibration. The variables considered in this simulation were particle size, *sand*, *clay*, *silt*, ρ_b, ρ_p, θ_s and a measured $\theta(h)$ point. This point was analyzed with any measurement between $\theta(0.5\ m)$ and $\theta(1.5\ m)$, according to the available data in the database.

- PTF1 of Splintex 2.0, uses the same principle as PTF2 of Splintex 1.0, with the same input configuration, but without including the optional measured $\theta(h)$ point. Instead, the value $\theta(3.3\ m)$ was estimated according to equation 6.

- PTF2 of Splintex 2.0 is based on the same principle as PTF2 of Splintex 1.0, with the same input information.

- Neuropack is a neural-network PTF that was trained using international data, with four hidden units to estimate parameters θ_r, α, n and m of equation 1, from the input data *sand*, *clay* and ρ_b.

- Rosetta is a neural-network that was trained using the U.S. and international data, with six hidden units for estimating the VGM parameters of the $K(\theta)$ equation from the input data *sand*, *silt*, *clay* and ρ_b.

Measures of RMSE of the analyzed PTFs for the estimation of water retention in the Brazilian and international data sets showed in Table 2. Splintex 2.0 performed clearly better than Splintex 1.0, which only yielded RMSE = 0.228 $m^3\ m^{-3}$ and r = 0.476, while PTF2 of Splintex 2.0 (simulation A) showed 0.082 $m^3\ m^{-3}$ and r = 0.805. The relative improvement over Splintex 1.0 is a reduction of two times the RMSE for the Brazilian database. However, for the international database, the results only showed small improvement, with RMSE value decreasing from 0.088 to 0.082 $m^3\ m^{-3}$ and r value increasing from 0.858 to 0.877.

The improvement, particularly for the Brazilian dataset, is due to the change in the constraint of the parameter θ_s used in the algorithm. In Splintex 1.0, this restriction was programmed as: "*if* $\theta_s > \phi$ *then* $\theta_s = \phi$". However, θ_s is run in Splintex 1.0 as a percentage of mass (%) yielding values larger than 1 ($\theta_s > 1$) for soils with extreme sand content, which is not realistic. This result was not previously identified by Silva et al. (2017a) and Silva et al. (2017b), neither by Reis et al. (2018), since their evaluated data sets were not composed by soils with the textural contents of the soils evaluated in this study.

Table 2: Volumetric soil water content [$\theta(h)$] using fitted-measured data and the parameters estimated by Splintex 1.0, Splintex 2.0, Neuropack and Rosetta for the evaluated Brazilian and international soils.

PTF	RMSE	ME	MAE	*r*
	$m^3\ m^{-3}$			-
	Brazilian database			
Splintex 1.0-PTF2	0.228	0.007	0.070	0.476^{**}
Splintex 2.0-PTF1-simA	0.097	0.037	0.079	0.816^{*}
Splintex 2.0-PTF1-simB	0.103	0.044	0.084	0.826^{*}
Splintex 2.0-PTF2-simA	0.082	-0.001	0.065	0.805^{*}
Splintex 2.0-PTF2-simB	0.084	0.010	0.067	0.813^{*}
Neuropack	0.072	-0.033	0.057	0.822^{*}
Rosetta	0.065	-0.016	0.046	0.815^{*}
	International database			
Splintex 1.0-PTF2	0.088	0.021	0.069	0.858^{*}
Splintex 2.0-PTF1-simA	0.100	0.044	0.082	0.841^{*}
Splintex 2.0-PTF1-simB	0.094	0.028	0.077	0.822^{*}
Splintex 2.0-PTF2-simA	0.085	0.007	0.070	0.854^{*}
Splintex 2.0-PTF2-simB	0.082	-0.003	0.067	0.877^{*}
Neuropack	0.058	-0.018	0.045	0.892^{*}
Rosetta	0.057	0.007	0.045	0.886^{*}

RMSE: root mean square error, ME: mean error, MAE: mean absolute error, *r*: coefficient of Pearson correlation, simA: results of the second column, considered to estimate parameters θ_r, α, n, and m, simB: results of the third column, considered to estimate parameters θ_s, θ_r, α, n and m, PTF1: without the input of the $\theta(h)$ point and PTF2: with the input of the $\theta(h)$ point, **: significant at P-value=0.02% and *: significant at P-value<0.001%.

Both output options of Splintex 2.0 were compared: simulation A (where three parameters were estimated) and simulation B (where four parameters were estimated). In terms of RMSE and MAE exhibited in table 2, for Splintex 2.0-PTF1-simA *versus* Splintex 2.0-PTF1-simB or for Splintex 2.0-PTF2-simA *versus* Splintex 2.0-PTF2-simB, the difference was not significant. This result indicates that to set parameter θ_s does not assure improvement in the SWRC estimation.

The inputs of Splintex 2.0 were also compared where in simulation A only particle-size distribution, ρ_b, ρ_p and θ_s were used and in simulation B the same variables and a measured $\theta(h)$ point was inserted as input. An improvement was noticed when Splintex 2.0-PTF2 was tested, since RMSE reduced from 0.103 to 0.082 m^3 m^{-3} for the Brazilian data set and from 0.100 to 0.082 m^3 m^{-3} for the international database.

The PTF models Rosetta, which has more hidden units and was trained using a larger data set, and Neuropack showed similar performance than Splintex 2.0 for the Brazilian database (Table 2). The values of RMSE between Rosetta and Neuropack were close for the international database (0.057 m^3 m^{-3} and 0.058 m^3 m^{-3}, respectively) but slightly better than Splintex-PTF2-simB. The three PTFs tend to underestimate the water content for the Brazilian database, as shown by the negative values of ME, whereas some versions of Splintex tends to overestimate them.

Both physical-empirical (Splintex 2.0) and neural-network (Neuropack and Rosetta) models presented acceptable measures of RMSE, varying from 0.065 to 0.103 m^3 m^{-3} for the Brazilian database and 0.057 to 0.10 m^3 m^{-3} for the international database. As expected, the performance of both Rosetta and Neuropack was better for the international database, since some of the data from the international database were used in their model calibration. However, the RMSE variation between Neuropack, Rosetta and Splintex 2.0-PTF2-simB was not large (0.065–0.082 m^3 m^{-3}) for the Brazilian database. Both Neuropack and Rosetta did not use the Brazilian database for their model calibration.

Medeiros et al. (2014) tested the performance of PTFs described by Tomasella et al. (2000), Vereecken et al. (1989) and Barros et al. (2010) for estimating the VGM parameters. They reported RMSE values ranging from 0.05 to 0.12 m^3 m^{-3} for 67 soil samples from the southeastern state of Pará, Brazil. The error measures of Medeiros et al. (2014) presented high variation, besides the number of samples may not be representative for the whole region of Brazil, and the RMSE results obtained in this study are smaller than the maximum values reported by them.

RMSE values between 0.053 to 0.065 m^3 m^{-3} were reported for Neuropack (Minasny and McBratney, 2002) and Rosetta (Zhang and Schaap, 2017). These errors were similar with the found results in this study for the international database, with Rosetta = 0.057 m^3 m^{-3} and Neuropack = 0.058 m^3 m^{-3}, except for Splintex 2.0-PTF2-simB (RMSE=0.082 m^3 m^{-3}).

As observed in figures 4 and 5, the estimates fell near the 1:1 line, with good accuracy for both databases. The estimates of Splintex 2.0 were strongly correlated with measured data (figure 4b) with similar values of RMSE obtained with Neuropack and Rosetta.

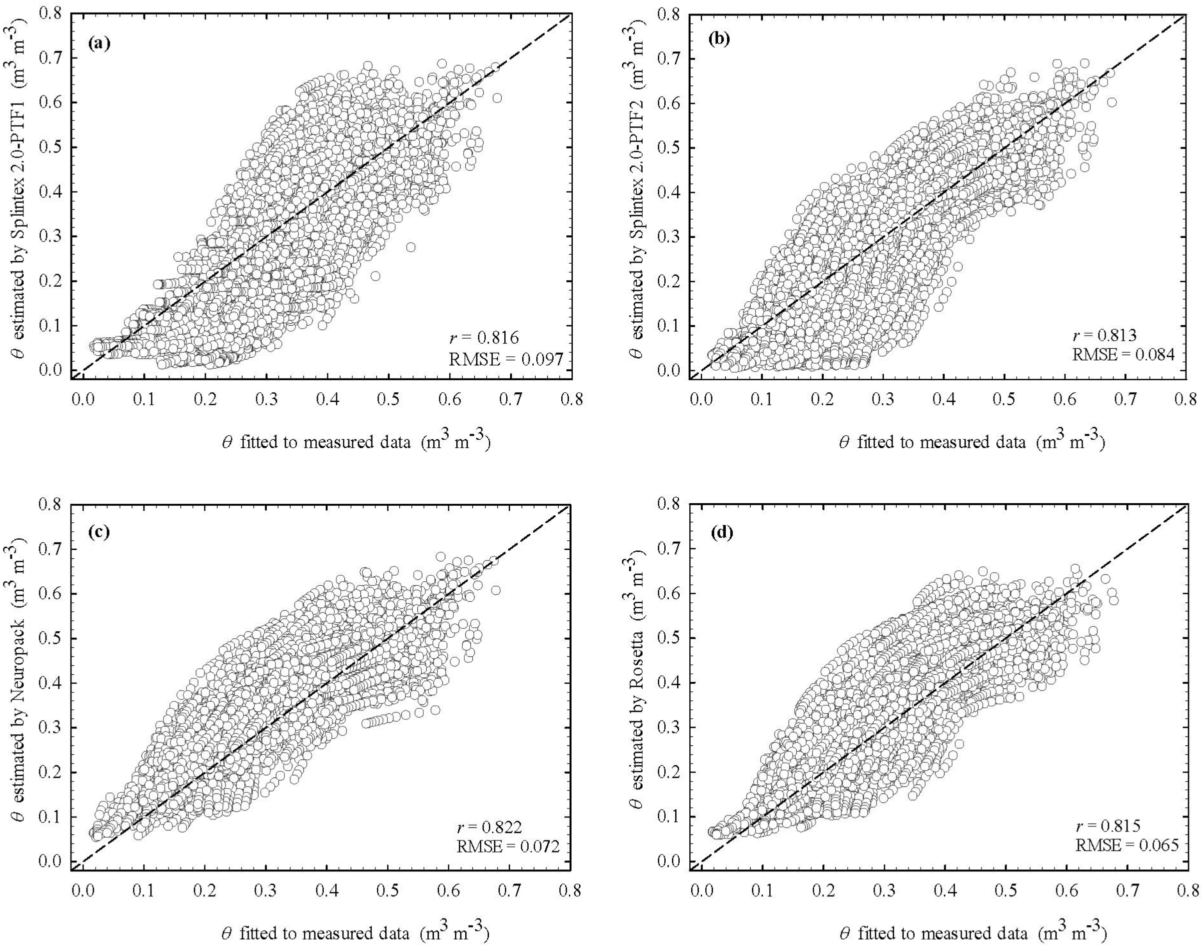

Figure 4 - Correlation between volumetric soil water content measured and estimated with PTFs for Brazilian database. (a) Splintex 2.0-PTF1-simA: results of the second column considered to estimate parameters θ_r, α, n and m, whereas θ_s was set as its measured value; (b) Splintex 2.0-PTF2-simB: results of the third column considered to estimate parameters θ_s, θ_r, α, n and m, and with the input of the $\theta(h)$ point; (c) Neuropack and (d) Rosetta.

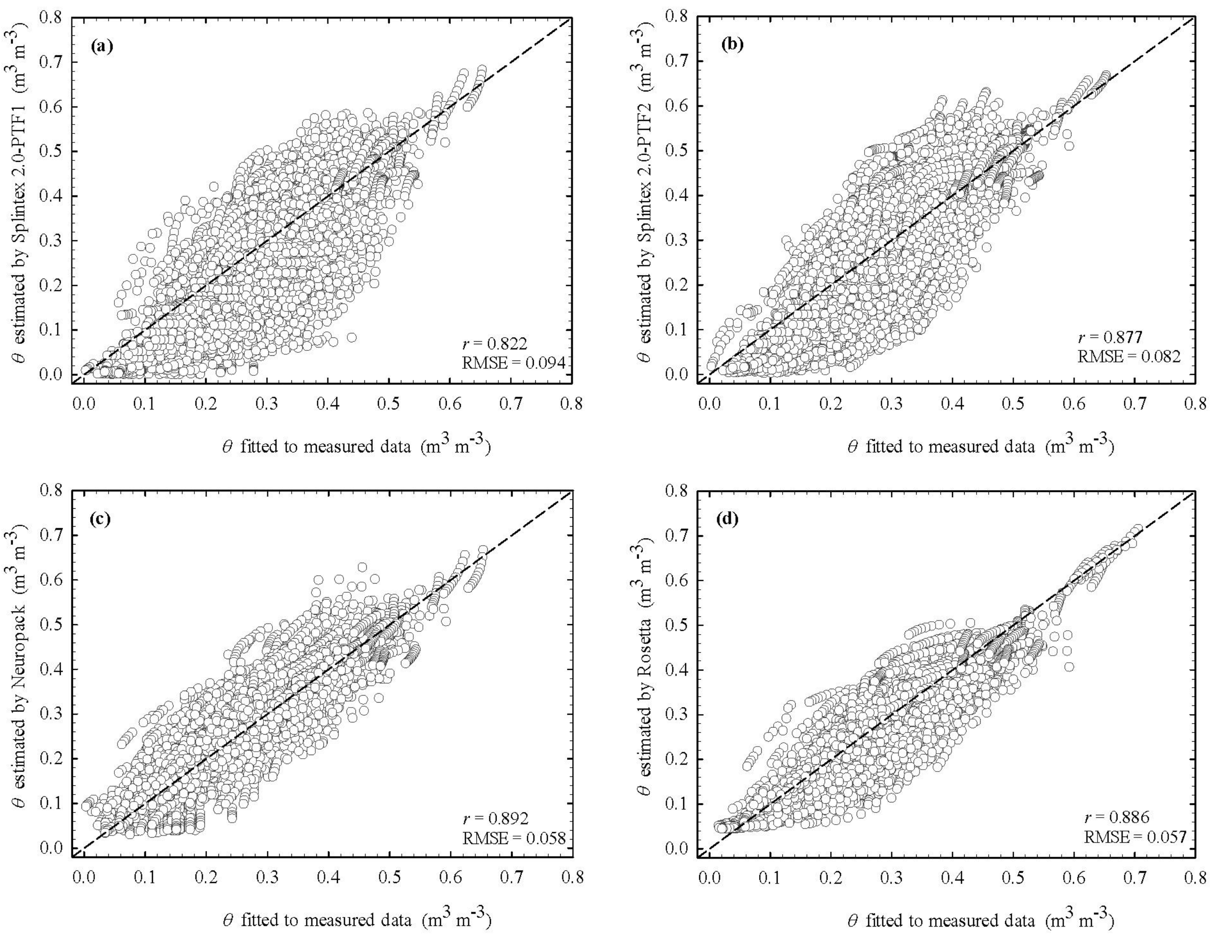

Figure 5 - Correlation between volumetric soil water content measured and estimated with PTFs for international database. (a) Splintex 2.0-PTF1-simB: results of the third column considered to estimate parameters θ_s, θ_r, α, n and m, and without the input of the $\theta(h)$ point; (b) Splintex 2.0-PTF2-simB: results of the third column considered to estimate parameters θ_s, θ_r, α, n and m, and with the input of the $\theta(h)$ point; (c) Neuropack and (d) Rosetta.

The patterns of RMSE measures were similar for both databases (Figure 6). The Splintex 2.0-PTF2, Neuropack and Rosetta models exhibited continuous RMSE values, with maximum h distribution between 0.4 and 1.0 m (Figure 6a). After that, RMSE becomes substantially small (typically 0.05 to 0.07 m^3 m^{-3}). The values presented in figure 6b were continuous for the Splintex 2.0-PTF2, Neuropack and Rosetta models.

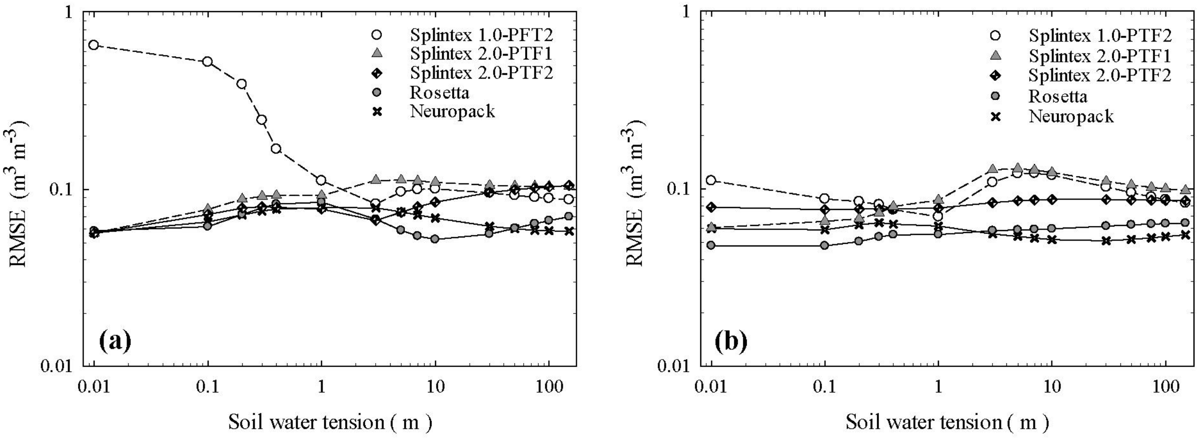

Figure 6 - Computed mean RMSE values for fifteen *h* values: 0.01, 0.1, 0.2, 0.3, 0.4, 1, 3, 5, 7, 10, 30, 50, 75, 100, and 150 m. (a) 750 samples of the Brazilian soils estimated with Rosetta, Neuropack, Splintex 1.0-PTF2, Splintex 2.0-PTF1, and Splintex 2.0-PTF2 with simulation A; (b) 380 samples of international soils estimated with Rosetta, Neuropack, Splintex 1.0-PTF2, Splintex 2.0-PTF1, and Splintex 2.0-PTF2 with simulation B.

Zhang and Schaap (2017) reported an improvement in their estimation of 0.074 to 0.039 m^3 m^{-3} when values of h of 3.3 and 150 m were used as inputs together with texture and ρ_b. Both Splintex 1.0 and 2.0 are flexible, allowing as additional input any h value between $\theta(0)$ and $\theta(150\ m)$.

3.5.4 Parameters distribution

A comparison between measured and estimated VGM parameters by various PTFs is shown in table 3. A high variation of the parameters α and n for both databases was observed. These are fitted parameters and their values are quite sensitive to the chosen criterion of fitting procedure (Wösten and van Genuchten, 1988). Difficulties in finding adequate PTFs for estimating parameters α and n have been reported by several other authors such as Wösten et al. (2001), Pachepsky and Rawls (2004), Silva et al. (2017a), and Zhang and Schaap (2017).

In regards to the Brazilian database, the found measured mean value of α is around 27 m^{-1}, whereas 8.13 m^{-1} was identified for the international database. Small values of α indicate few changes in θ as h becomes large, which is generally more likely in fine-grained and unstructured soils (Hodnett and Tomasella, 2002). Mean values of α were underestimated in all scenarios, except for Splintex 1.0. In contrast, small overestimations on the mean values of n were noticed, varying from 1.16 to 2.43 m^3 m^{-3} for the Brazilian database and 1.23 to 2.44 m^3 m^{-3} for the international database.

Table 3: Fitted VGM parameters using measured data and estimated VGM parameters by Splintex 1.0, Splintex 2.0, Rosetta, and Neuropack models for Brazilian and international database.

Parameters		Measured	Splintex 1.0-PTF2	Splintex 2.0-PTF1		Splintex 2.0-PTF2		Neuropack	Rosetta
				simA	simB	simA	simB		
	Brazilian database								
	max	0.683	11.68	0.686	0.697	0.686	0.691	0.686	0.655
θ_s ($m^3 m^{-3}$)	mean	0.481	0.588	0.457	0.468	0.457	0.468	0.457	0.443
	min	0.269	0.302	0.301	0.306	0.301	0.294	0.301	0.326
	range	0.414	11.38	0.385	0.391	0.385	0.397	0.385	0.329
	max	0.381	0.393	0.333	0.139	0.513	0.179	0.172	0.167
θ_r ($m^3 m^{-3}$)	mean	0.160	0.159	0.098	0.016	0.087	0.006	0.064	0.106
	min	0.000	0.004	0.000	0.000	0.000	0.000	0.000	0.058
	range	0.381	0.389	0.333	0.139	0.513	0.179	0.172	0.109
	max	200.0	149.3	17.98	20.92	32.66	43.47	21.21	2.801
α (m^{-1})	mean	27.01	4.87	3.483	4.903	2.568	3.425	4.509	1.175
	min	0.266	0.389	0.502	0.669	0.140	0.452	0.690	0.434
	range	199.7	148.9	17.48	20.25	32.52	43.01	20.52	2.366
	max	9.140	5.896	20.39	4.755	4.760	2.804	1.360	2.222
n	mean	1.426	2.429	2.207	1.510	1.867	1.344	1.163	1.343
	min	1.045	1.134	1.068	1.047	1.053	1.042	1.059	1.199
	range	8.096	4.762	19.33	3.708	3.707	1.763	0.302	1.023
	International database								
	max	0.654	1.443	0.668	0.958	0.668	0.952	0.668	0.655
θ_s ($m^3 m^{-3}$)	mean	0.395	0.444	0.428	0.454	0.428	0.443	0.428	0.392
	min	0.202	0.019	0.200	0.302	0.200	0.298	0.200	0.276
	range	0.452	1.424	0.468	0.655	0.468	0.654	0.468	0.379
	max	0.312	0.330	0.262	0.285	0.285	0.285	0.181	0.166
θ_r ($m^3 m^{-3}$)	mean	0.064	0.094	0.062	0.033	0.043	0.065	0.044	0.085
	min	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.046
	range	0.312	0.330	0.261	0.285	0.284	0.285	0.181	0.119
	max	328.8	138.0	17.09	40.76	34.45	48.37	20.10	3.705
α (m^{-1})	mean	8.127	2.216	2.418	1.730	1.137	2.433	3.285	1.238
	min	0.075	0.260	0.063	0.129	0.049	0.542	0.700	0.366
	Range	328.8	137.8	17.03	40.64	34.40	47.82	19.40	3.339
	max	15.00	5.630	4.767	4.124	4.514	4.124	1.455	3.714
n	mean	1.792	2.447	2.349	1.707	1.997	2.274	1.231	1.524
	min.	1.020	1.175	1.030	1.080	1.045	1.116	1.078	1.178
	range	13.98	4.455	3.736	3.044	3.469	3.008	0.377	2.536

Max: maximum, Min: minimum, θ_s: saturated water content, θ_r: residual water content, α and n: fitting parameters of equation 1, SimA: results of the second column considered to estimate parameters θ_r, α, n and m, SimB: results of the third column considered to estimate parameters θ_s, θ_r, α, n and m, PTF1: without the input of the $\theta(h)$ point and PTF2: with the input of the $\theta(h)$ point.

The parameter θ_s was significantly larger for the Brazilian database (Table 3) together with the greatest mean value of ϕ (Table 1). Estimates showed small underestimation in the θ_s values for the data set from Brazil, except with Splintex 1.0. On average, θ_s presented an measured value of 0.481 $m^3 m^{-3}$ for the Brazilian database, against 0.443 to 0.468 $m^3 m^{-3}$

estimated with PTFs. For the international database, measured θ_s was equal to 0.395 m^3 m^{-3}, against 0.392 to 0.454 m^3 m^{-3} estimated with the PTFs.

In contrast to θ_s, θ_r is only a fitting parameter. Both databases presented values of θ_r near or equal to zero, with little scatter, in general all PTFs underestimated the mean values of θ_r, which tended to have a narrower distribution in comparison with the measured data. The mean θ_r for the Brazilian database was 0.16 m^3 m^{-3}, compared to only 0.064 m^3 m^{-3} for international soils. For both databases θ_r exceeded 0.3 m^3 m^{-3}, a value suggested as a fitting constraint by Hodnett and Tomasella (2002).

Zhang and Schaap (2017) and Reis et al. (2018) found small correlations between PTFs estimated and data-fitted parameters, but when estimated parameters were used to yield θ, a good performance was noticed. Moreover, Barros et al. (2013) reported that the good performance of a PTF for describing $\theta(h)$ depends on the combination of all VGM parameters.

3.5.5 Evaluation of the water content at field capacity

The correlation between θ_{fc} values assumed as $\theta(3.3\ m)$ and estimated with PTFs is presented in figure 7. For the Brazilian database (Figure 7a), the found results are:

- Splintex 2.0-PTF2-simA, RMSE = 0.07 m^3 m^{-3} with r = 0.74,
- Neuropack, RMSE = 0.08 m^3 m^{-3} with r = 0.72,
- Rosetta, RMSE = 0.07 m^3 m^{-3} with r = 0.73.

For international database (Figure 7b), the results were slightly better:

- Splintex-PTF1-simB = 0.07 m^3 m^{-3} with r = 0.83,
- Neuropack = 0.06 m^3 m^{-3} with r = 0.84,
- Rosetta = 0.06 m^3 m^{-3} with r = 0.82.

The obtained results were similar, with high accuracy and precision for both databases. These results are in line with the overall finding of PTFs:

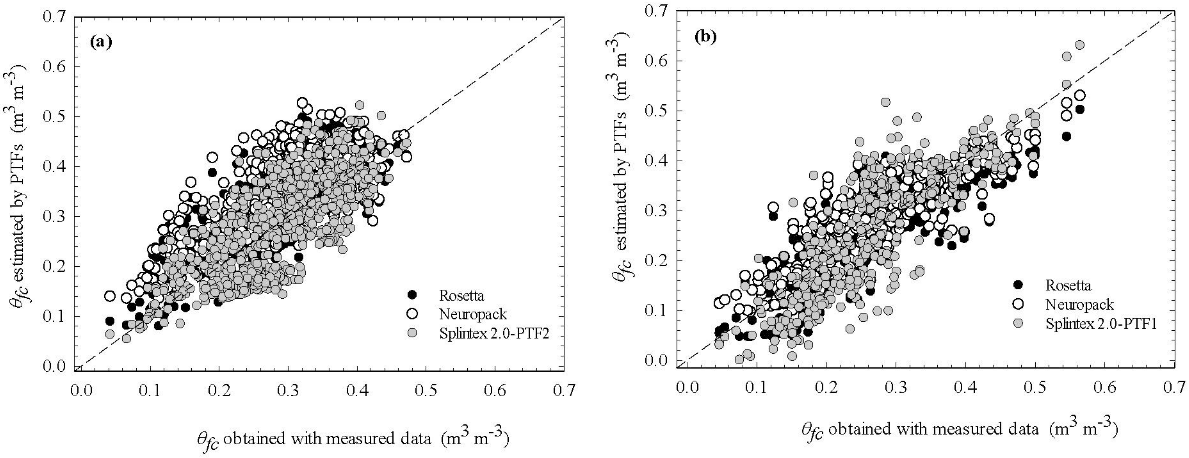

Figure 7 - Correlation between soil water content at field capacity with measured-fitted data according to VGM model and the one estimated with PTFs. (a) Rosetta, Neuropack, and Splintex 2.0-PTF2-simA estimates for Brazilian soils and (b) Rosetta, Neuropack, and Splintex-PTF1-simB estimates for international soils.

Regardless of the *h* value used for determining θ_{fc}, the error interval tends to remain the same, according to the RMSE distribution based on *h* values (Figure 6). Similar results were found by Turek et al. (2018), who evaluated the performance of PTF developed by Saxton et al. (1986) to estimate θ_{fc} as $\theta(3.3\ m)$, reporting *r* from 0.74 to 0.78 for 60 soil samples located in Piracicaba, Brazil.

All PTFs were quite similar in the estimations and are recommendable. Based on Pearson's correlation coefficient, no estimation method exceeded $r = 0.84$, therefore Splintex 2.0 is an alternative PTF model for estimating θ_{fc}.

3.6 CONCLUSIONS

We presented in this study a new PTF model (Splintex 2.0) which was programmed in C ++ language with a user-friendly interface for estimating the parameters of the VGM equation of SWRC. Splintex 2.0 is based on physical principles, does not require any calibration and can be applied to any porous medium. In regards to Splintex 1.0, a RMSE reduction of 2 times was found for the Brazilian database. Splintex 2.0, Rosetta, and Neuropack models presented similar accuracies for the Brazilian database with high precision for estimating the soil water content. For the international database, the accuracy of Rosetta and Neuropack was larger in comparison with the one of Splintex 2.0. This better performance was expected because those PTFs used part of this international database (UNSODA and GRIZZLY) in their calibrations. Furthermore, the found results of correlation and accuracy show Splintex 2.0 also as a viable PTF for the international database. With regards to field capacity, the performance of all PTFs was similar to estimate this point with high accuracy and precision for both databases.

3.7 REFERENCES

Arruda, F.B., Zullo, J.J., Oliveira, J.B., 1987. Soil parameters for the calculation of the available water based on soil texture. **Revista Brasileira de Ciência do Solo**. 11, 11–15.

Arya, L.M., Paris, J.F., 1981. A physico-empirical model to predict the soil moisture characteristic from particle-size distribution and bulk density data. **Soil Science Society of America Journal**. 45, 1023–1030.

Arya, L.M., Richeter, J.C., Davidson, S.A., 1982. A comparison of soil moisture characteristic predicted by the Arya-Paris model with laboratory-measured data. **Agristars Technology Resport**. Sm-L1-04247, JSC-17820, NASA-Johson Space Center, Houston, TX.

Arya, L.M., Leij, F.J., Van Genuchten, M.Th., Shouse, P.J., 1999a. Scaling Parameter to Predict the Soil Water Characteristic from Particle-Size Distribution Data. **Soil Science Society of America Journal**. 63, 510–519.

Arya, L.M., Leij, F.J., Shouse, P.J., Van Genuchten, M.Th., 1999b. Relationship between the Hydraulic Conductivity Function and the Particle-Size Distribution. **Soil Science Society of America Journal**. 63, 1063–1070.

Arya, L.M., Heitman, J.L., 2015. A Non-Empirical Method for Computing Pore Radii and Soil Water Characteristics from Particle-Size Distribution. **Soil Science Society of America Journal**. 79, 1537–1544.

Armindo, R.A., Wendroth, O., 2016. Physical soil structure evaluation based on hydraulic energy functions. **Soil Science Society of America Journal**. 80:1167–1180.

Barros, A.H.C., Van Lier, Q.J., Maia, A.H.N., Scarpare, F.V., 2013. Pedotransfer functions to estimate water retention parameters of soils in northeastern Brazil. **Revista Brasileira de Ciência do Solo**. 37, 379–391.

Bouma J., 1989. Using soil survey data for quantitative land evaluation. **Advanced Soil Science**. 9, 177–213.

Chaney, N.W., Minasny, B., Herman, J.D., Nauman, T.W., Brungard, C., Morgan, C.L.S., McBratney, A.B., Wood, E.F., Yimam, Y.T., 2019. POLARIS soil properties: 30-meter probabilistic maps of soil properties over the contiguous United States. **Water Resources Research**. 1–53.

Haghverdi, A., Öztürk, H.S., Cornelis, W.M., 2014. Revisiting the pseudo continuous pedotransfer function concept: Impact of data quality and data mining method. **Geoderma**. 227, 31–38.

Haverkamp, R.C., Zammit, F., Bouraoui, K., Rajkai, J.L.A., Heckman, N., 1997. GRIZZLY, Grenoble Soil Catalogue. Soil survey of field data and description of particle size, soil water retention and hydraulic conductivity functions. **Laboratoire d'Étude des Transfers en**

Hydrologie et Environnement, LTHE, UMR5564, CNRS, INPG, ORSTOM, UJF, BP 53, 38041 Grenoble Cédex 09, xz France.

Hodnett, M.G., Tomasella, J., 2002. Marked differences between van Genuchten soil water-retention parameters for temperate and tropical soils: a new water-retention pedotransfer function developed for tropical soils. **Geoderma**. 108, 155–180.

McBratney, A.B., Minasny, B., Cattle, S.R., Vervoort, R.W., 2002. From pedotransfer functions to soil inference systems. **Geoderma**. 109, 41–73.

Medrado, E., Lima, J.E.W., 2014. Development of pedotransfer functions for estimating water retention curve for tropical soils of the Brazilian Savanna. **Geoderma Regional**. 1:59–66.

Minasny, B., McBratney, A.B., 2002. The Neuro-m method for fitting neural network parametric Pedotransfer function. **Soil Science Society of America Journal**. 66, 352–361.

Mualem, Y., 1976. A new model for predicting the hydraulic conductivity of unsaturated porous media. **Water Resource Research**. 12:513–522.

Minasny, B., McBratney, A.B., Bristow, K.L., 1999. Comparison of different approaches to the development of pedotransfer functions for water-retention curves. **Geoderma**. 93, 225–253.

Michelon, C.J., Carlesso, R., Oliveira, Z.B., Kniesi, A.E.K., Petry, M.T., Martins, J.D., 2010. Funções de pedotransferência para estimativa da retenção de água em alguns solos do Rio Grande do Sul. **Ciência Rural**. 40, 848–853.

Nemes, A., Schaap, M.G., Leij, F.J., Wosten, J.H.M., 2001. Description of the unsaturated soil hydraulic database UNSOSA version 2.0. **Journal of Hydrology**. 251, 151–162.

Oliveira, L.B., Ribeiro, M.R., Jacomine, P.K.T., Rodrigues, J.J.V., Marques, F.A., 2002. Funções de pedotransferência para predição da umidade retida a potenciais específicos em solos do estado de Pernambuco. **Revista Brasileira de Ciência do Solo**. 26, 315–323.

Ottoni, M.V., Ottoni, F.T.B., Schaap, M.G., Lopes-Assad, M.L.R.C., Rotunno, F.O.C., 2018. Hydrophysical database for Brazilian soils (HYBRAS) and pedotransfer functions for water retention. **Vadose Zone Journal**. 170095, 1–17. doi:10.2136/vzj2017.05.0095.

Pachepsky, Y.A., Rawls, W.J., 2004. Development of Pedotransfer Functions in Soil Hydrology. **In: Developments in Soil Science 30**. Elsevier, Amsterdam. 525p.

Prevedello, C.L., Loyola, J.M.T., 2002. Modelo para estimar as propriedades hidráulicas de meios porosos a partir da curva granulométrica. **Congresso Brasileiro de Mecânica dos Solos e Engenharia Geotécnica**, São Paulo, 2002. ABMS, Anais. São Paulo, pp. 467–472.

Prevedello, C.L., Armindo, R.A., 2016. Generalization of the Green-Ampt theory for horizontal infiltration into homogeneous soil. **Vadose Zone Journal**. 15, 1–10.

Reis, A.M.H., Armindo, R.A., Duraes, M.F., Lier., Q.J.V., 2018. Evaluating pedotransfer functions of the Splintex model. **European Journal of Soil Science**. 69, 685–697.

Richards, L.A., Weaver, L.R., 1944. Moisture retention by some irrigated soils as related to soil moisture tension. **Journal Agricultural Research**. 69, 215–235.

Reichert, J.M., Albuquerque, J.A., Kaiser, D.R., Reinert, D.J., Urach, F.L., Carlesso, R., 2009. Estimation of water retention and availability in soils of Rio Grande do Sul. **Revista Brasileira de Ciência do Solo**. 33, 1547–1560.

Ribeiro, K.D., Nascimento, J.M.S., Gomes N.M., Lima, L.A., Menezes, S.M., 2007. Relações matemáticas entre porosidade drenável e condutividade hidráulica do solo saturado. **Revista Brasileira de Engenharia Agrícola e Ambiental**. 11, 600–606.

Rudiyanto, Sakai, M., Van Genuchten, M.T., Alazba, A.A., Setiawan, B.I. and Minasny, B., 2015. A complete soil hydraulic model accounting for capillary and adsorptive water retention, capillary and film conductivity, and hysteresis. **Water Resources Research**, 51, 8757–8772.

Saxton, K.E., Rawls, W.J., Romberger, J.S., Papendick, R.I., 1986. Estimating generalized soil-water characteristics from texture. **Soil Science Society of America Journal**. 50, 1031–1036.

Schaap, M.G., Leij, F.J., Van Genuchten, M.Th., 2001. Rosetta: a computer program for estimating soil hydraulic parameters with hierarchical pedotransfer functions. **Journal of Hydrology**. 251, 163–176.

Silva, A.C., Armindo, R.A., Brito, A.S., Schaap, M.G., 2017a. Splintex: A physically-based pedotransfer function for modeling soil hydraulic functions. **Soil Tillage Research**. 174, 261–272.

Silva, A.C., Armindo, R.A., Brito, A.S., Schaap, M.G., 2017b. An assessment of pedotransfer function performance for the estimation of spatial variability of key soil hydraulic properties. **Vadose Zone Journal**. 16, 1–10.

Soil Survey Staff., 1999. Soil Taxonomy: A Basic System of Soil Classification for Making and Interpreting Soil Surveys, Second Edition. **Natural Resources Conservation Service. U.S**. Department of Agriculture Handbook 436, Washington, DC.

Tomasella, J., Hodnett, M.G., 1998. Estimating soil water retention characteristics from limited data in Brazilian Amazonia. **Soil Science Society of America Journal**. 163, 190–202.

Tomasella, J., Hodnett, M.G., Rossato., L., 2000. Pedotransfer functions for the estimation of soil water retention in Brazilian soils. **Soil Science Society of America Journal**. 64, 327–338.

Tomasella, J., Hodnett, M.G., Cuartas, L.A., Nobre, A.D., Waterloo, M.J., Oliveira, S.M., 2008. The water balance of an Amazonian micro-catchment: the effect of interannual variability of rainfall on hydrological behaviour. **Hydrological Processes**. 22, 2133–2147.

Turek, M.E., Armindo, R.A., Wendroth, O., Santos, I., 2018. Criteria for the estimation of field capacity and their implications for the bucket type model. **European Journal Soil Science**. 69, 1–8.

Van Genuchten, M.Th., 1980. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. **Soil Science Society of America Journal**. 44, 892–897.

Jong Van Lier, Q.D., Wendroth, O., Van Dam, J., 2015. Prediction of winter wheat yield with the SWAP model using pedotransfer functions: An evaluation of sensitivity, parameterization and prediction accuracy. **Agricultural Water Management on Science Direct**. 154, 29–42.

Jong Van Lier, Q.D., 2017. Field capacity, a valid upper limit of crop available water. **Agricultural Water Management on Science Direct**. 193, 214–220.

Van Looy, K., Bouma, J., Herbst, M., Koestel, J., Minasny, B., Mishra, U., Vereecken, H., 2017. Pedotransfer functions in Earth system science: Challenges and perspectives. **Reviews of Geophysics**. 55, 1199–1256.

Vaz, C.M.P., Iossi, M.F., Naime, J.M., Macedo, A., Reichert, J.M., Reinert, D.J. et al. 2005. Validation of the Arya and Paris water retention model for Brazilian soils. **Soil Science Society of America Journal**. 69, 577–583.

Vereecken, H., Feyen, J., Maes, J., 1989. Estimating the soil moisture retention characteristic from particle size distribution, bulk density and carbon content. **Soil Science**. 148, 389–403.

Wösten, J.H.M., Van Genuchten, M.Th., 1988. Using Texture and Other Soil Properties to Predict the Unsaturated Soil Hydraulic Functions. **Soil Science Society of America Journal**. 52, 1762–1770.

Wösten, J.H.M., Pachepsky, Ya.A., Rawls, W.J., 2001. Pedotransfer functions: bridging the gap between available basic soil data and missing soil hydraulic characteristics. **Journal of Hydrology**. 251, 126–150.

Zhang, Y., Schaap, M.G., Guadagnini, A., Neuman, S.P., 2016. Inverse modeling of unsaturated flow using clusters of soil texture and Pedotransfer functions. **Water Resources Research**. 52, 1–14.

Zhang, Y., Schaap, M., 2017. Weighted recalibration of the Rosetta Pedotransfer model with improved estimates of hydraulic parameter distributions and summary statistics (Rosetta3). **Journal of Hydrology**. 547, 39–53.

4 CHAPTER III: USING SPLINTEX 2.0 TO ESTIMATE THE SOIL HYDRAULIC CONDUCTIVITY CURVE MEASURED WITH INSTANTANEOUS PROFILE METHOD

4.1 ABSTRACT

Soil hydraulic conductivity curve (SHCC) is a fundamental function in hydrological and environmental studies. Measuring SHCC is a difficult and onerous task and often unfeasible in large-scale monitoring, therefore pedotransfer functions (PTFs) have been an alternative way for estimating SHCC. In this study, the novel model Splintex 2.0 is presented as an auxiliary tool to estimate unsaturated soil hydraulic conductivity (K) as a function of water content (θ) based on the particle size distribution (PSD). Splintex 2.0 estimates the function $K(\theta)$ assuming that soil pores can be represented by equivalent capillary tubes and that the water flow rate is a function of pore size distribution. Then, the estimated data are fitted to the SHCC described by the van Genuchten (1980)-Mualem (VGM) parameters. The goodness-of-fit of Splintex 2.0 was evaluated for data from 198 soil samples. Each data set contains measured information of textural composition, particle and bulk density, $K(\theta)$ values, and the optional values for saturated water content and total porosity. The performance of estimates was computed through Pearson correlation coefficient (r), mean error (ME), and square root mean error (RMSE) measures. The comparison between estimated and measured SHCC for the four textures analyzed showed a mean RMSE of $log_{10}[K(\theta)]$ of 1.17, ranging from 0.77 to 1.22, exhibiting good performance for PTFs purposes.

Keywords: Pedotransfer function. Soil hydraulic permeability. Particle size distribution.

4.2 RESUMO

A curva de condutividade hidráulica do solo (CCHS) é uma função essencial em estudos hidrológicos e ambientais. Medir CCHS geralmente é uma tarefa onerosa e inviável, principalmente no monitoramento em grande escala, assim funções de pedotransferência (FPTs) têm sido alternativamente uma opção para estimar a CCHS. Apresenta-se o modelo Splintex 2.0, que estima a condutividade hidráulica do solo não saturado (K) em função do teor de água (θ) obtido com base na distribuição de tamanho de partículas (DP). O Splintex 2.0 estima $K(\theta)$ assumindo que os poros do solo podem ser representados por tubos capilares equivalentes e que o fluxo de água é função do tamanho do poro. O desempenho do Splintex 2.0 para estimar CCHS com base nos parâmetros de van Genuchten (1980)-Mualem (VGM) foi avaliado em 198 amostras de solo por meio da correlação de Pearson (r), erro médio (ME) e raiz quadrada do erro médio (RMSE). Cada conjunto de dados contém informações de composição textural, densidade do solo e das partículas, $K(\theta)$ e um opcional teor de água do solo na saturação ou porosidade total. A comparação entre a CCHS estimada e medida, dentre os quatro grupos texturais analisados, mostrou RMSE de $log_{10}[K(\theta)]$ médio de 1,17, variando de 0,77 a 1,22, indicando bom desempenho do modelo.

Palavras-chave: Função de pedotransferência. Permeabilidade hidráulica do solo. Distribuição de frequência de partículas.

4.3 INTRODUCTION

Although numerical models have become increasingly more sophisticated, the success and reliability of these models depend on accurate information about the parameters of hydrological systems (Schaap and Leij, 2000). The quantification of soil hydraulic functions is of great importance to model hydrological processes. The hydraulic conductivity function is one of the essential tools for modelling flow in unsaturated and saturated soils, which allows the understanding of issues related to irrigation and internal drainage in soil profile (Rahmati et al., 2018) as well as relationships between water-plant and surface/groundwater (Ghanbarian et al., 2015; Vereecken et al., 2016; Elhakeem et al, 2018).

The soil hydraulic conductivity curve (SHCC) often presents high spatial and temporal variability (Sarki et al., 2014; Silva et al., 2017b; Elhakeema et al., 2018) because it is extensively controlled by several soil properties, such as soil texture and structural behavior. These properties include macropores or fractured rock (Schaap and van Genuchten, 2006; van Genuchten and Pachepsky, 2011; García-Gutiérrez et al., 2018), which are also affected by temperature and soil management (Elhakeem et al., 2018; Hirmas et al., 2018). On the other hand, measuring soil hydraulic functions, such as SHCC, is a difficult, time consuming and costly task. As an alternative, SHCC are usually estimated through models that employ physical or empirical relationships between other soil hydraulic functions and key-variables from more readily available data. These models, denominated pedotransfer functions (PTFs), were firstly introduced in soil science by Bouma (1989) and aimed to unify various terms used in the literature to describe the meaning of transforming existing information into nonexistent soil data.

Several PTFs were developed worldwide, in which soil texture, bulk density and other key-variables are used as input to estimate soil water retention curve (SWRC) and saturated hydraulic conductivity (K_s) (Vereecken et al., 1989; Silva et al., 2017a; Zhang and Schaap, 2017; Reis et al., 2018). However, fewer alternatives are available for the SHCC estimation (Saxton et al., 1986; Schuh and Bauder, 1986; Vereecken et al., 1990). Despite their importance, most of the PTFs do not incorporate structural soil information (e.g., aggregation and pores connectivity), which may cause reduction of accuracy in the SHCC estimates near to the saturation point (Schaap and Leij, 2000). PTFs are somehow limited in terms of geographic region, climate, geological and soil management conditions from where they were originally developed. In order to improve the performance of PTFs, Ottoni et al. (2019) and Weynants et al. (2009) suggested that soil hydraulic parameters can be better estimated by incorporating structure variables into the PTFs, meaning that PTFs developed based on physical models could yield more accurate estimates.

Splintex is a physical-based PTF model that estimates soil hydraulic parameters to build the hydraulic functions SWRC and SHCC. In the first version, Splintex 1.0 estimates the SWRC parameters based on van Genuchten (1980)-Mualem (VGM) equation and K_s, based on the textured-PTF developed by Rodas (1970) for soils from Lima, Peru, South America. By using K_s and SWRC parameters, soil hydraulic functions as water retention [$h(\theta)$], unsaturated hydraulic conductivity [$K(\theta)$], specific water capacity [$C(\theta)$], and hydraulic diffusivity [$D(\theta)$] were derived by Silva et al. (2017a) and Silva et al. (2017b). Our studies have shown that Splintex model can be applied to any porous medium without requiring model calibration (Silva et al., 2017a; Silva et al., 2017b; Reis et al., 2018).

Splintex 2.0 is an improved-developed model to estimate VGM parameters of SWRC and SHCC. Regarding the estimation of $K(\theta)$, this second version applies a compilation of information described by Arya et al. (1981), Arya et al. (1999b), and Arya et al. (2015) to quantify $K(\theta)$ data. This step is based on the assumption that the soil pores can be represented by equivalent capillary tubes and that the water flow rate can be represented as a function of pore size distribution (Arya et al., 1999a).

This study aims to analyze the performance of the new-developed version of the Splintex model (Splintex 2.0) in the SHCC estimation. The specific aims are to explore Splintex 2.0 in the estimation of VGM parameters for different soil texture groups, *(i)* to investigate its performance in the estimation of $K(\theta)$ under different bulk density values, and *(ii)* to evaluate its performance in the estimation of $K(\theta)$ in the near-saturation range.

4.4 MATERIAL AND METHODS

4.4.1 Database

A data set with 198 sample points were selected from the UNSODA database (Nemes et al., 2001), aiming to evaluate the performance of Splintex 2.0 in the estimation of the function unsaturated hydraulic conductivity [$K(\theta)$]. The criterion for sample selection combines data availability of $K(\theta)$, textural composition (according to USDA classification), bulk density (ρ_b), and solid-particle density (ρ_p) values that refer to measured saturated water content (θ_s) or total porosity (ϕ), whose descriptive statistics are presented in table 1.

Among the several methods available for $K(\theta)$ estimation, $K(\theta)$ data from sampling points were measured by the instantaneous profile method under field conditions (Nemes et al., 2001). In this method, θ was measured by neutron probes and K was determined by using tension infiltrometers and solving Richards equation, considering internal drainage after flood irrigation with zero flux condition at the soil surface (Hillel et al., 1972).

Table 1: Summary statistics of soil properties used to estimate the function $K(\theta)$ with Splintex 2.0.

Summary	Texture (% mass)			ρ_b	ρ_p	ϕ
	Sand	Silt	Clay	kg dm^{-3}		%
	Unsoda database					
Maximum	96.4	87.0	62.0	1.83	2.77	69.8
Mean	63.7	20.9	15.4	1.51	2.65	43.2
Minimum	1.00	1.00	1.00	0.72	2.58	24.5
SD	26.6	18.9	13.5	0.18	0.02	8.9
CV (%)	41.8	90.4	87.7	11.8	0.67	20.5

SD: standard deviation, CV: coefficient of variation, ρ_b: bulk density, ρ_p: particle density and ϕ: total porosity.

The data set covers a wide soil textural variety according to USDA classification (Figure 1, Soil Survey Staff, 1999). The textural composition has predominance of sand (25.8%), followed by sandy loam (16.7%), loamy sand (15.7%), sandy clay loam (12.6%), clay loam (7.6%), silt loam (7.6%), loam (7.1%) clay (3.5%), silty clay loam (2.5%), sandy clay (0.5%), and silt (0.5%).

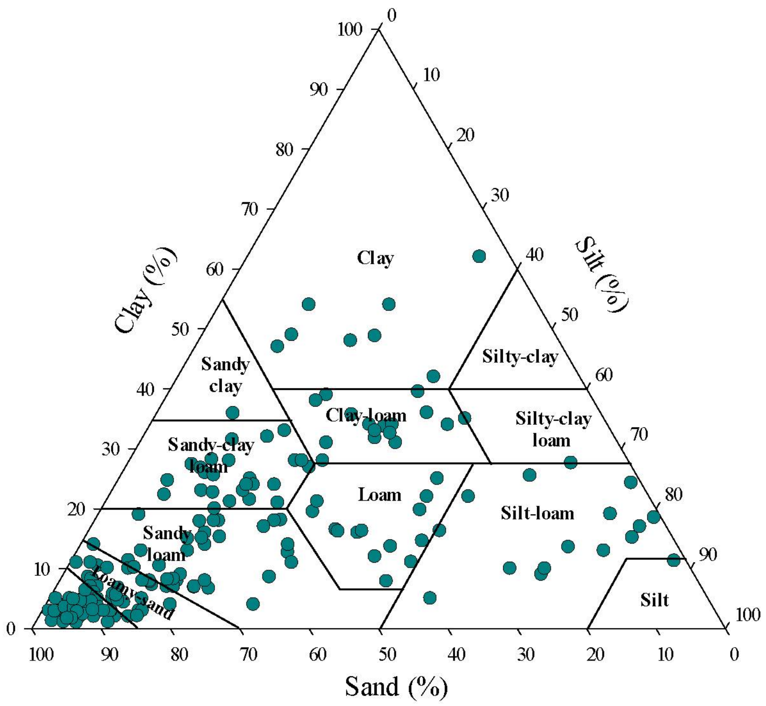

Figure 1 - The USDA triangle of textural classes (Soil Survey Staff, 1999) of the 198 data sets used to estimate the VGM parameters of function $K(\theta)$.

4.4.2 Estimation of unsaturated hydraulic conductivity

Splintex 2.0 is a computer program able to estimate VGM parameters of both functions SWRC and SHCC by means of parametric PTFs. By means of the Mualem's (1976) equation, van Genuchten (1980) yielded the following closed-form expression for SHCC:

$$K(\theta)=K_s \Theta^{\lambda}\left[1-\left(1-\Theta^{1/m}\right)^m\right]^2 \quad , \quad \Theta=\frac{\theta-\theta_r}{\theta_s-\theta_r} \tag{1}$$

in which K is the unsaturated hydraulic conductivity (cm d^{-1}) as a function of θ, the volumetric soil water content (m^3 m^{-3}). K_s is a fitted matching at saturation point (cm d^{-1}), Θ is the effective degree of saturation (m^3 m^{-3}), θ_r and θ_s are respectively the residual and saturated water content (m^3 m^{-3}), and λ and $m=1-1/n$ are empirical parameters related with the connectivity of pores and curve shape.

4.4.3 Development of PTFs to estimate unsaturated hydraulic conductivity

The structure of Splintex 2.0 holds a set of physical equations described by Arya et al. (1981), Arya et al. (1999b), and Arya et al. (2015) to estimate $K(\theta)$ data. The first principle is the calculation of θ_i from the particle size distribution (PSD), as contribution of each fraction of the soil wetting, as

$$\theta_i \approx \phi S_w \sum_{j=0}^{j=i} w_j; \quad i=1, 2, ..., N \tag{2}$$

in which ϕ is the soil total porosity (m^3 m^{-3}), S_w is the ratio of measured saturated water content (θ_s) to theoretical porosity and w_i is the solid mass of the i-th fraction (kg kg^{-1}).

In the calculation of θ_i, PSD was standardized for 16 classes of particle diameters: 2, 4, 6, 8, 10, 20, 40, 50, 60, 80, 100, 200, 400, 600, 800, 1000 µm. So, the PSD curve was divided into N fractions and then the pore volume associated with the solid mass for each fraction, based on the assumption that ρ_b and ρ_p were applied to each fraction. Pore volumes were then progressively summed up and converted into θ_i of the i-*th* fraction. Further information about PSD on water content scale can be seen in Arya and Paris (1981) and Arya et al. (1999a).

The second principle is based on the assumption that the soil pores can be represented by equivalent capillary tubes and that the flow rate behaves as function of PSD. Based on the above simplifications made by Arya et al. (1999b), the volumetric flow rate (Q_i) is the sum of the individual saturated pore flow rates within the pore fraction of a particular soil sample, in which the flow occurs according to Hagen-Poiseuille's law for capillary flow (Hillel, 1971).

$$Q_i \approx q_i N_i \tag{3}$$

in which q_i is the volumetric flow rate for a single pore (m^3 s^{-1}) and N_i is the number of pores in the i-*th* pore size fraction.

The volumetric flow rate for a single pore (q_i) is computed as follows:

$$q_i \approx \frac{\pi R_i^x}{S\eta} \frac{\rho_w g \Delta H}{L} \tag{4}$$

in which R_i is the mean pore radius (m) for the i-*th* pore fraction, ρ_w is the density of water (kg m^{-3}), g is the gravity acceleration (m s^{-2}), η is the viscosity of water (kg m^{-1} s^{-1}), x and the shape factor S are dimensionless parameters, L is the length of the flow path (m) and ΔH is the hydraulic tension difference across the sample length in the direction of flow (m).

Although the pore water flux is affected by many factors, such as the pore-size distribution, tortuosity, shape, roughness and degree of interconnectivity of the pores as well as fluid properties (van Genuchten and Pachepsky, 2011; Zhang and Schaap, 2019). Arya et al. (1999b) followed a pragmatic approach (except for pore size) and assumed a unitary gradient combining all factors into a single empirical variable. As a result, equation 4 is modified to

$$q_i \approx c R_i^x \tag{5}$$

in which c and x are empirical parameters described in table 2. A more complete description of the $K(\theta)$ estimation is provided in Arya et al. (1999b).

The radius of the pores (R_i) can be calculated with the methodology presented in Arya et al. (2015). These authors proposed a formulation for computing pore radii from routinely available PSD, ρ_b, ρ_p data for most soils, thus eliminating the need for unknown empirical parameters. R_i is then obtained as follows:

$$R_i = \sqrt{\frac{0.0717 \phi \, w_i}{\tau_i^{4/3} \mu_i \, \rho_b}} \tag{6}$$

in which R_i is the pore radius for a given fraction of particles on the PSD curve (m), τ_i is the number of spherical particles that can be formed using the fraction solid mass, ρ_b is the soil bulk and particle densities (kg m^{-3}) and μ_i is the mean particle radius for the fraction (m), considering packing of spherical particles.

For flow under a unitary gradient, equations 3, 4, 5, and 6 can be combined to formulate the function $K(\theta_i)$, resulting in:

$$K(\theta_i)=\frac{1}{A_b}\sum_{j=1}^{j=i}\left(cR_j^x\right)N_j\,;\quad i=1,2,...,N \tag{7}$$

in which N_j is the number of pores in the i-th pore fraction, exposed at the cross-section area, R_j is the i-th pore radius fraction (m), A_b is the sample cross-sectional area (m^2) given by $A_b = (1/\rho_b)^{2/3}$.

4.4.4 Performance evaluation criteria

The R environment was used to develop the descriptive statistics in order to evaluate patterns between the assessed soil properties and $K(\theta)$ parameters obtained with measured and estimated data with Splintex 2.0. Summary statistics (e.g., minimum, maximum, medium, standard deviation and coefficient of variation) were used to describe the distribution of soil properties. The Pearson correlation coefficient (r), mean error (ME) and root mean square error (RMSE) were computed in order to analyze the goodness of fit of $K(\theta)$ estimates yielded by Splintex 2.0, as follows:

$$r=\frac{Cov\left[K_e,K_m\right]}{S_{K_e}S_{K_m}} \tag{8}$$

$$ME=\frac{1}{N}\sum_{i=1}^{n}\left[log_{10}(K_e)-log_{10}(K_m)\right] \tag{9}$$

$$RMSE=\sqrt{\frac{1}{N}\sum_{i=1}^{n}\left[log_{10}(K_e)-log_{10}(K_m)\right]^2} \tag{10}$$

in which K_m is the i-th measured variable, K_e is the i-th estimated variable, Cov is the covariance, N is the number of measures, S_{ke} and S_{km} are standard deviation of measured and estimated values of hydraulic conductivity. The mean results were evaluated for each textural group as well as for the complete data set.

4.5 RESULTS AND DISCUSSION

4.5.1 Splintex 2.0 model

The description of the variation of the key-soil information used in the estimation with Splintex 2.0 are presented in table 1. The size of the particles in the data set is quite diverse, from low sand content to high clay content. The values of sand and silt presented maximum values with high values of coefficient of variation (CV) in relation to the clay fraction.

The mean values of the parameters θ_s, m and K_s were close when the fitted VGM parameters (Equation 1) were compared with the ones estimated by Splintex (Table 2). The variation of the mean K_s on the logarithmic scale was similar between the measured and estimated data for the four texture groups analyzed in this study.

Table 2: Mean fitted VGM parameters of equation 1 obtained with measured and estimated data with Splintex 2.0 for 198 samples from UNSODA data set.

Soil texture classes	Summary	Experimental parameters θ_s	θ_r	m	λ	$\log_{10}(K_s)$	Splintex 2.0 parameters θ_s	θ_r	m	λ	$\log_{10}(K_s)$
		$m^3 m^{-3}$		-	-	cm d^{-1}	$m^3 m^{-3}$		-	-	cm d^{-1}
All	Maximum	0.91	0.54	0.99	16.9	2.99	0.81	0.20	0.97	1.51	2.74
	Mean	0.42	0.10	0.59	1.70	1.60	0.45	0.01	0.49	0.51	1.51
	Minimum	0.12	0.00	0.04	0.05	-1.01	0.26	0.00	0.21	-0.79	0.17
	SD	0.14	0.13	0.29	2.79	0.91	0.10	0.02	0.18	0.22	0.44
Sands	Maximum	0.92	0.44	0.99	7.27	2.99	0.71	0.16	0.97	1.51	2.18
(I)	Mean	0.41	0.08	0.65	1.37	1.69	0.42	0.01	0.55	0.50	1.64
	Minimum	0.12	0.00	0.04	0.00	-1.00	0.26	0.00	0.32	-0.79	0.82
	SD	0.14	0.11	0.29	1.76	0.98	0.07	0.01	0.18	0.26	0.21
Loams	Maximum	0.78	0.32	0.93	10.4	2.41	0.74	0.20	0.52	0.56	1.94
(II)	Mean	0.44	0.14	0.43	1.74	1.50	0.49	0.01	0.41	0.53	0.94
	Minimum	0.30	0.00	0.11	0.10	-0.55	0.33	0.00	0.30	0.34	0.23
	SD	0.11	0.13	0.26	2.71	0.69	0.09	0.03	0.07	0.04	0.40
Silts	Maximum	0.68	0.43	0.93	16.9	2.20	0.81	0.14	0.40	0.55	2.74
(III)	Mean	0.47	0.14	0.47	3.84	1.19	0.61	0.01	0.31	0.53	1.94
	Minimum	0.33	0.00	0.12	0.09	0.45	0.46	0.00	0.21	0.48	0.96
	SD	0.10	0.16	0.27	5.95	0.54	0.13	0.03	0.06	0.02	0.36
Clays	Maximum	0.91	0.54	0.93	12.9	2.33	0.69	0.06	0.52	0.56	2.16
(IV)	Mean	0.51	0.22	0.51	2.47	1.37	0.52	0.05	0.32	0.53	0.85
	Minimum	0.27	0.00	0.14	0.10	0.41	0.38	0.03	0.22	0.46	0.17
	SD	0.17	0.19	0.29	4.25	0.62	0.11	0.01	0.09	0.02	0.54

Parameters	Empirical parameters of equation 7 for four soil textures: Sands *(I)*	Loams *(II)*	Silts*(III)*	Clays*(IV)*
log (c)	1.849	2.647	0.482	-0.488
x	3.999	4.258	3.602	3.506

θ_s: saturated water content, θ_r: residual water content, c and x: parameters of the function $K(\theta)$ described in equation 7, λ and m: $1\text{-}1/n$, K_s: fitted matching point at saturation, SD: standard deviation, *(I)* sandy, loamy sand, sandy loam, sandy clay loam; *(II)* loamy, clay loam; *(III)* silty loam, silt and *(IV)* clayey, sandy clay, silty clay loam.

However, a little underestimate of the mean values of K_s estimated for loamy and clayey texture groups was identified. This difference of the real may be due to the sensitivity of the parameters to the fitting procedure. In addition, data sets comprising a limited range of measured SHCC for the clayey class may also lead to convergence problems of VGM parameter estimates (van Genuchten et al., 1991).

The results obtained for the parameter λ presented variation for both fitting procedures comparing with the commonly used value of λ = 0.5. This value was proposed by Mualem (1976) as an optimal value for a set of 45 different texture samples. However, Schuh and Cline (1990) report large variation of λ, ranging from -8.73 to 14.80, with increased variation for smaller mean particle diameters in a data set of 75 samples, located at the northern region of the United States. The same behavior was noticed in this study, in which the highest values of λ were observed for particles from clay and silt groups. Schaap and Leij (2000) found that λ was often negative in most of the VGM fitting procedures, with an ideal value of -1 for λ.

4.5.2 Splintex 2.0 performance for the SHCC estimation in the near-saturation range

The values of saturated hydraulic conductivity (K_s) fitted with measured data and estimated with Splintex 2.0 are presented in figure 2a, where moderate correlation with values of r = 0.48 is presented. Regarding the distribution of measured *versus* estimated values of K_s (Figure 2b), the behavior was similar among the 198 samples. Sampling points from 100 to 140 presents an overestimation of K_s whereas an underestimation is identified for the other points.

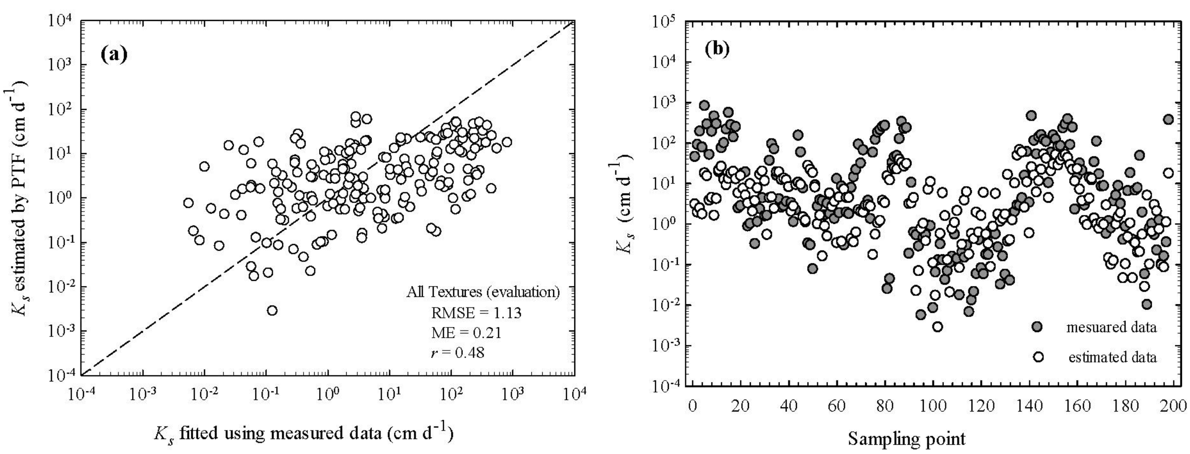

Figure 2 - Comparison of measured and estimated K_s for 198 sample points of the UNSODA database. (a) correlation of the measured *versus* estimated K_s and (b) distribution of measured and estimated K_s.

This difference between K_s described in figure 2 may be related to certain limitations of equation 1. Schaap and van Genuchten (2006) report the limitation of VGM equation involving the shape of the hydraulic conductivity function near saturation, especially of structured media (i.e., macroporous soils or unsaturated fractured rock). As a matter fact, the performance of equation 1 for fitting measured $K(\theta)$ data is often questioning. Schaap and Leij (2000) described the presence of macropores or fractures that dominate the flow regime close to the soil saturation, and micropores that control the flow with the matrix. The matrix flow would thus be active at all pressures, whereas the macropore flow dominates only near saturation and becomes insignificant at some relatively small tensions. This result indicates that equation 1 could be modified to better describe SHCC in both wet and dry ranges (Schaap and van Genuchten, 2006).

The accuracy of Splintex 2.0 in the K_s estimation (RMSE = 1.13, ME = 0.21) was similar to the results presented by Minasny and McBratney (2000) for a structural model (their K9 model) calibrated with 462 samples from Australian soils (RMSE = 1.15, EM = -0.166). On the other hand, it was slightly higher than that reported by Ottoni et al. (2019), which is based on texture and ρ_b ranging from 0.86 to 0.90 for RMSE. Schaap et al. (2001) described for an only texture-based PTF (H2 of the Rosetta model) a RMSE of 0.72 and ME of -0.001 for 1,306 soils used in the calibration. However, all models mentioned above were calibrated to a specific database and only estimates K_s and SWRC parameters, as Splintex 1.0. Splintex 2.0 is built-off a physical-based model for the SHCC estimation, applicable to any porous medium without requiring model calibration (Silva et al., 2017a), according to accuracy and precision presented in table 3.

Table 3: Mean performance of estimates of equation 1 yielded by Splintex 2.0 for each soil textural group.

Soil texture Classes	*N*	RMSE	ME	*r*
Sands *(I)*	140	1.22	- 0.14	0.862
Loams *(II)*	29	1.11	- 0.34	0.824
Silts *(III)*	16	1.09	0.08	0.801
Clays (IV)	13	0.77	- 0.27	0.859
All	198	1.17	- 0.16	0.852

RMSE: root mean square error; ME: mean error; *r*: coefficient of Pearson correlation; *N*: number of samples; *(I)* sandy, loamy sand, sandy loam, sandy clay loam; *(II)* loamy, clay loam; *(III)* silty loam, silt and *(IV)* clayey, sandy clay, silty clay, silty clay loam.

The positive linear correlations between the results of $K(\theta)$ yielded with measured data and estimated with Splintex 2.0 are presented in table 3 and figure 3. The estimates of SHCC were strongly correlated with measured data for the sands group (r = 0.862). Although the correlation analysis for the clays group did not show the best values for r, the greatest accuracy was observed for this group (RMSE = 0.77 and ME = -0.16). However, SHCC was very well estimated with r = 0.852 for all soil samples for the four texture groups together. Arya et al. (1999b) evaluated 16 soil samples from the UNSODA database and achieved great performance for the SHCC estimation, with mean logarithm RMSE ranging from 0.487 to 1.562, and r = 0.89.

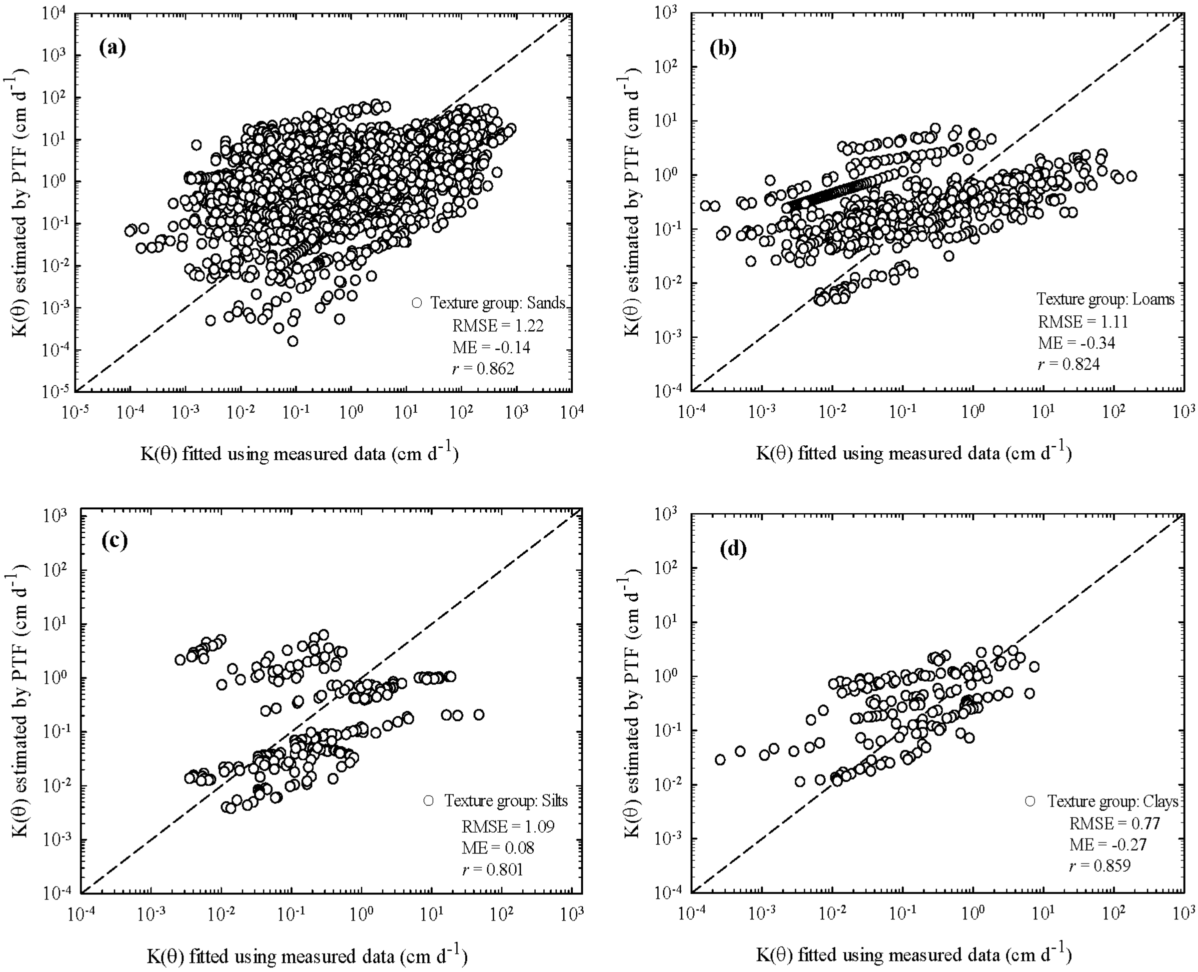

Figure 3 - SHCC fitted with measured data and estimated with Splintex 2.0 for the four texture groups of UNSODA. (a) *Sands*: sandy, loamy sand, sandy loam, and sandy clay loam; (b) *Loams*: loamy, clay loam; (c) *Silts*: silty loam, and silt and (d) *Clays*: clayey, sandy clay, silty clay, and silty clay loam.

4.5.3 Estimation of SHCC under different bulk density values

Splintex 1.0 estimates K_s based on the textural-PTF developed by Rodas (1970) for soils from Peru. This means that K_s is fixed even when the value of a structural variable of the soil, e.g., ρ_b, is varied. On the other hand, two soil structure variables were inserted into Splintex 2.0 code [ρ_b and θ_s (or ϕ)] in this estimation.

The fitted parameters of the VGM model and the function SHCC estimated with Splintex 2.0 for different ρ_b values are presented in figure 4 and table 4. As it can be seen, *K(θ)* behavior decreases with ρ_b increasing. This is an advantage compared with texture-based-PTFs, which do not describe spatial and temporal variation for *K(θ)* in the same area. Thereby, the estimates of Splintex 2.0 tend to manifest the structural difference, whereas Splintex 1.0 would yield only constant values of K_s. For this reason, estimates yielded by Splintex 1.0 were not presented in figure 4. Ottoni et al. (2019) described that the adoption of soil structural variables, e.g., effective porosity, could benefit in the estimation of K_s, presenting better performance compared to PTF models that are only based on texture.

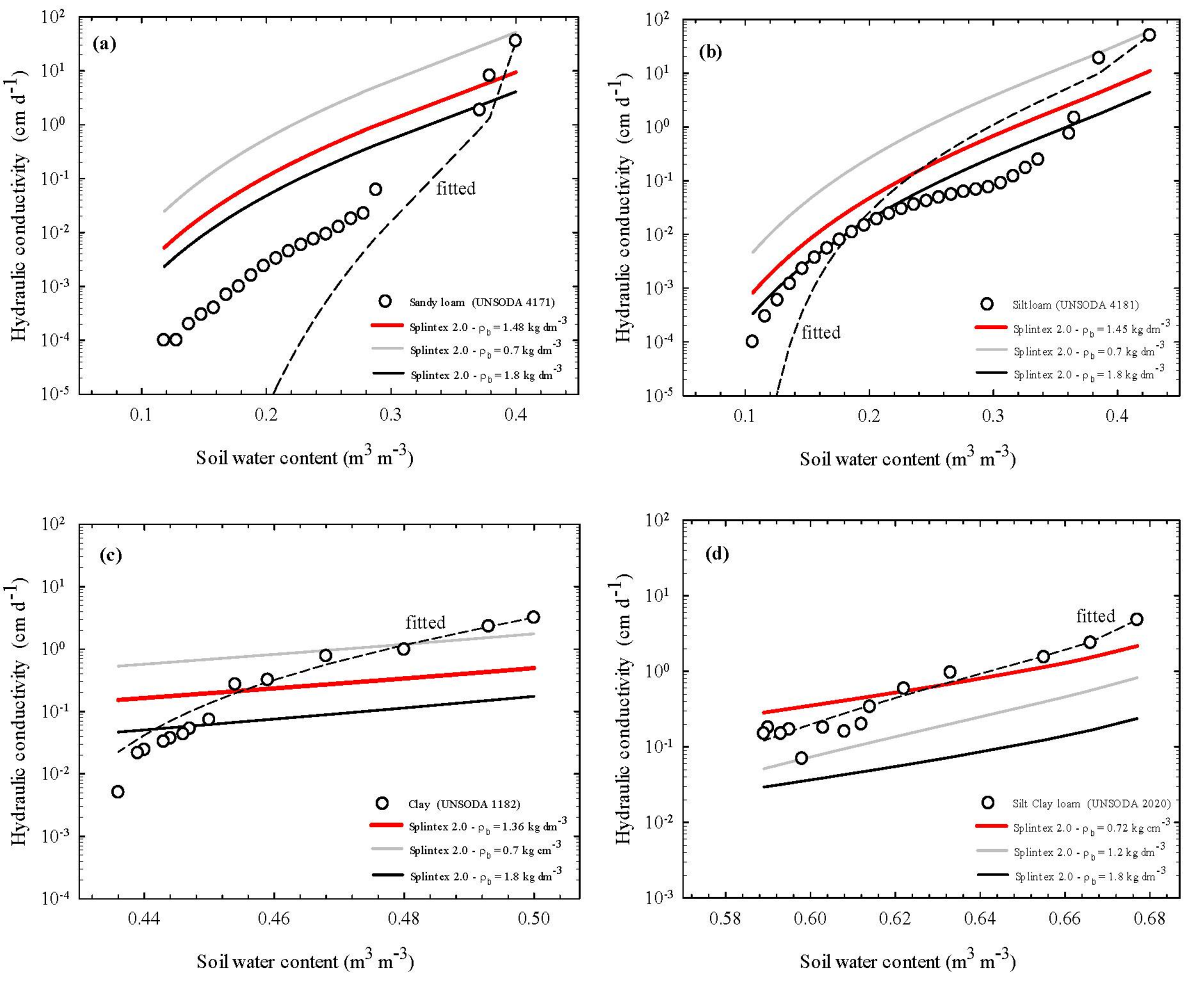

Figure 4 - Soil hydraulic conductivity as function of water content using measured data, fitted and estimated with Splintex 2.0 for different bulk density values: (a) sandy, (b) silt loamy, (c) clayey and (d) silty clay loam.

Therefore, management variables that are related to soil structure (e.g., profile development, horizon, land use, and the roots presence) could be added to enhance the PTFs (Weynants et al., 2009). Furthermore, the covariance between estimates throughout a transect could be added (Wendroth et al., 2006) in order to improve the estimates. The authors argue that the quantification of the spatial covariance behavior of pairs of variables to obtain efficient schemes of coregionalization is essential for a better understanding of the processes underlying the soil hydraulic properties.

Table 4: VGM parameters of the hydraulic conductivity curve estimated with Splintex 2.0 and fitted to measured data and their summarized statistical results.

UNSODA Code	Fitted parameters of VGM equation to measured data					r	RMSE
	θ_s (m^3 m^{-3})	θ_r (m^3 m^{-3})	m	λ	$\log_{10}[K_s$ (cm d^{-1})]		
4171_*Sandy l.*	0.400	0.113	0.196	0.202	1.53	0.983	1.566
4181_*Silt l.*	0.426	0.105	0.455	0.541	1.70	0.975	1.667
1182_*Clay*	0.509	0.418	0.768	0.479	0.72	0.996	0.261
2020_*Silt c. l.*	0.677	0.496	0.569	0.50	0.68	0.997	0.157
Mean	0.503	0.283	0.497	0.431	1.16	0.987	0.912
	Splintex 2.0 Estimated parameters of VGM equation						
4171_*Sandy l.*	0.452	0.005	0.405	0.531	1.75	0.861	1.546
4181_*Silt l.*	0.463	0.005	0.361	0.532	1.78	0.950	1.659
1182_*Clay*	0.552	0.006	0.364	0.555	0.51	0.981	0.715
2020_*Silt c. l.*	0.694	0.004	0.253	0.538	1.03	0.983	0.313
Mean	0.540	0.005	0.346	0.539	1.27	0.943	1.058

Sandy *l.*: Sandy loam, Silt *l.*: Silt loam, Silt *c. l.*: Silt clay loam, r: Pearson correlation coefficient, RMSE: root mean square error, θ_s: saturated water content, θ_r: residual water content, λ and m: 1-1/n, K_s: fitted matching point at saturation.

The correlation matrix (Table 5) for all data set shows that most variables have significant correlations ranging from 0.0001 to 0.982 (absolute values). K_s estimates had positive correlation with ϕ and negative with ρ_b, demonstrating the applicability of Splintex 2.0 to the analysis of the soil porous space, through the interpretation of the VGM parameters (e.g., θ_s, λ and K_s). Small values of ρ_b enhance pore space and therefore, potentially, emphasize the conductive path for water flow. Likewise, negative correlations were also found for θ_r, in this case, smaller θ_r values effectively increase the hydraulic activity of the porous space (Schaap and Leij, 2000).

Table 5: Linear correlation matrix among soil properties (input) and *K(θ)* parameters (output) estimated with Splintex 2.0 and fitted parameters from experimentally measured SHCC data for 198 samples of the UNSODA database.

		Input data						Fitted to measured data					Splintex 2.0				
		Clay	Silt	Sand	ρ_b	ρ_p	ϕ	θ_s	θ_r	m	λ	K_s	θ_s	θ_r	m	λ	K_s
Input data	Clay	1	**0.345**	**-0.752**	**-0.353**	0.024	**0.327**	*0.192*	**0.397**	**-0.328**	0.057	**-0.356**	**0.344**	0.182	**-0.465**	0.073	*-0.193*
	Silt	-	1	**-0.879**	**-0.347**	-0.053	**0.567**	0.156	*0.185*	**-0.359**	*0.230*	**-0.403**	**0.586**	0.113	**-0.569**	0.100	*0.196*
	Sand	-	-	1	**0.424**	0.025	**-0.565**	*-0.207*	**-0.332**	**0.419**	*-0.191*	**0.464**	**-0.587**	-0.172	**0.636**	-0.108	-0.039
	ρ_b	-	-	-	1	0.176	**-0.664**	**-0.363**	-0.023	0.175	-0.080	*-0.201*	**-0.668**	**-0.388**	**0.310**	0.039	**-0.333**
	ρ_p	-	-	-	-	1	-0.108	-0.081	-0.032	-0.032	-0.032	0.043	-0.108	-0.154	0.045	0.017	0.000
	ϕ	-	-	-	-	-	1	**0.317**	**0.257**	-0.153	0.031	**0.300**	**0.982**	**0.254**	**-0.429**	0.040	**0.272**
Fitted to measured data	θ_s	-	-	-	-	-	-	1	**0.282**	*0.209*	-0.097	0.085	**0.319**	0.021	**-0.305**	0.037	0.072
	θ_r	-	-	-	-	-	-	-	1	0.172	**-0.298**	-0.104	**0.257**	0.066	*-0.220*	0.040	-0.107
	m	-	-	-	-	-	-	-	-	1	0.091	**0.389**	*-0.169*	-0.101	**0.284**	-0.076	-0.043
	λ	-	-	-	-	-	-	-	-	-	1	-0.041	0.042	-0.064	-0.017	-0.040	0.021
	K_s	-	-	-	-	-	-	-	-	-	-	1	**-0.299**	-0.090	**0.244**	*-0.225*	-0.020
Splintex 2.0	θ_s	-	-	-	-	-	-	-	-	-	-	-	1	**0.262**	**-0.432**	0.039	**0.269**
	θ_r	-	-	-	-	-	-	-	-	-	-	-	-	1	-0.117	-0.058	*0.198*
	m	-	-	-	-	-	-	-	-	-	-	-	-	-	1	**-0.254**	-0.091
	λ	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1	-0.039
	K_s	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1

θ_s: saturated water content, θ_r: residual water content, ρ_b: bulk density, ρ_p: particle density, ϕ: total porosity, λ and m: 1-1/n and K_s: fitted matching point at saturation, bold values, significant at P-value<0.1%; italic, significant at P-value<1.0%; underlined, significant at P-value<5% and other values, not significant.

4.6 CONCLUSIONS

In this study, the performance of Splintex 2.0 for estimating VGM parameters that compose the hydraulic conductivity curve (SHCC) for different texture groups was evaluated. Splintex 2.0 provided very close mean values of VGM parameters fitted to measured data. For the four texture groups analyzed, the SHCC was well estimated with r = 0.852 and RMSE = 1.17. In addition, we evaluated the performance of Splintex 2.0 to estimate the saturated hydraulic conductivity (K_s). The results showed moderate correlation (r = 0.48) and similar distribution among the 198 sample points. Regarding the first version (Splintex 1.0), where K_s is estimated only based on texture data, Splintex 2.0 unlikely has in its code a physical-based model that is sensitive to the variation of bulk density, total porosity and saturated water content, yielding estimates that can contribute to the modelling and understanding of the water dynamics in soil vadose zone.

4.7 REFERENCES

Arya, L.M., Paris, J.F., 1981. A physico-empirical model to predict the soil moisture characteristic from particle-size distribution and bulk density data. **Soil Science Society of America Journal**. 45, 1023–1030.

Arya, L.M., Leij, F.J., Van Genuchten, M.Th., Shouse, P.J., 1999a. Scaling Parameter to Predict the Soil Water Characteristic from Particle-Size Distribution Data. **Soil Science Society of America Journal**. 63, 510–519.

Arya, L.M., Leij, F.J., Shouse, P.J., Van Genuchten, M.Th., 1999b. Relationship between the Hydraulic Conductivity Function and the Particle-Size Distribution. **Soil Science Society of America Journal**. 63, 1063–1070.

Arya, L.M., Heitman, J.L., 2015. A Non-Empirical Method for Computing Pore Radii and Soil Water Characteristics from Particle-Size Distribution. **Soil Science Society of America Journal**. 79, 1537–1544.

Bouma J., 1989. Using soil survey data for quantitative land evaluation. **Advanced Soil Science**. 9, 177–213.

Elhakeem, M., Papanicolaou, A.N.T., Wilson, C.G., Chang, Yi-Jia, Burras, L., Abban, B., Wysocki, D.A., Wills, S., 2018. Understanding saturated hydraulic conductivity under seasonal changes in climate and land use. **Geoderma**. 315, 75–97.

García-Gutiérrez, C., Pachepsky, Ya, Martín, M.A., 2018. Technical note: Saturated hydraulic conductivity and textural heterogeneity of soils. **Hydrology and Earth System Sciences**. 22, 3923–3932.

Ghanbarian, B., Taslimitehrani, V., Dong, G., Pachepsky, Ya., 2015. Scale-Dependent Pedotransfer Functions Reliability for Estimating Saturated Hydraulic Conductivity. **Journal of Hydrology**. 528, 127–137.

Hillel, D. 1971. Soil and water: Physical principles and processes. **Academic Press**, New York.

Hillel, D., Krentos, V.D., Stylianou, Y., 1972. Procedure and test of an internal drainage method for measuring soil hydraulic conductivity in situ. **Soil Science**.114, 395–400.

Hirmas, D.R., Giménez, D., Nemes, A., Kerry, R., Brunsell, N.A. and Wilson, C.J., 2018. Climate induced changes in continental-scale soil macroporosity may intensify water cycle. **Nature**. 561, 100–103.

Minasny, B., and McBratney, A.B., 2000. Evaluation and development of hydraulic conductivity Pedotransfer functions for Australian soil. **Australian Journal of Soil Research**. 38, 905–26.

Mualem, Y., 1976. A new model for predicting the hydraulic conductivity of unsaturated porous media. **Water Resource Research**. 12:513–522.

Nemes, A., Schaap, M.G., Leij, F.J., Wosten, J.H.M., 2001. Description of the unsaturated soil hydraulic database UNSOSA version 2.0. **Journal of Hydrology**. 251, 151–162.

Ottoni, M.V., Ottoni, F.T.B., Schaap, M.G., Lopes-Assad, M.L.R.C., Rotunno, F.O.C., 2018. Hydrophysical database for Brazilian soils (HYBRAS) and pedotransfer functions for water retention. **Vadose Zone Journal**. 95, 1–17.

Ottoni, M.V., Ottoni, T.B., Lopes-Assad, M.L.R.C., Rotunno, O.C., 2019 Pedotransfer functions for saturated hydraulic conductivity using a database with temperate and tropical climate soils. **Journal of Hydrology**. 575, 1345–1358.

Rahmati, M., Weihermüller, L., Vanderborght, J., 2018. Development and analysis of the Soil Water Infiltration Global database. **Earth System Science Data**. 10, 1237–1263.

Reis, A.M.H., Armindo, R.A., Duraes, M.F., Lier., Q.J.V., 2018. Evaluating pedotransfer functions of the Splintex model. **European Journal of Soil Science**. 69, 685–697.

Rodas, A., 1970. Determinación de la conductividad hidráulica em muestras de suelo inalterada. Lima, **CENDRET**. 118p.

Saxton K.E., Rawls, W.J., Romberger, J.S., and Papendick, R.I., 1986. Estimating generalized soil water characteristics from texture. **Soil Science Society of America Journal**. 50, 1301–1036.

Sarki, A., Mirjat, M.S., Mahessar, A.A., Kori, S.M., Qureshi, A.L., 2014. Determination of Saturated Hydraulic Conductivity of Different Soil Texture Materials. **Journal of Agriculture and Veterinary Science** (IOSR-JAVS), 7(12). ver IV:56-62.

Schuh, W.M., and J.W. Bauder. 1986. Effect of soil properties on hydraulic conductivity-moisture relationships. **Soil Science Society of America Journal**. 50, 848–855.

Schuh, W.M., and R.L. Cline. 1990. Effect of soil properties on unsaturated hydraulic conductivity pore-interaction factors. **Soil Science Society of America Journal**. 54, 1509–1519.

Schaap, M.G; Leij, F.J., 2000. Improved Prediction of Unsaturated Hydraulic Conductivity with the Mualem-van Genuchten Model. **Soil Science Society of America Journal**. 64, 843–851.

Schaap, M.G, Leij, F.J., Van Genuchten, MTh., 2001. ROSSETA: computer program for estimating soil hydraulic parameters with hierarchical pedotransfer functions. **Journal of Hydrology**. 251, 163–176.

Schaap, M.G; Van Genuchten, M.Th., 2006.A Modified Mualem–van Genuchten Formulation for Improved Description of the Hydraulic Conductivity Near Saturation. **Vadose Zone Journal**. 5, 27–34.

Silva, A.C., Armindo, R.A., Brito, A.S., Schaap, M.G., 2017a. Splintex: A physically-based pedotransfer function for modeling soil hydraulic functions. **Soil Tillage Research**. 174, 261–272.

Silva, A.C., Armindo, R.A., Brito, A.S., Schaap, M.G., 2017b. An assessment of pedotransfer function performance for the estimation of spatial variability of key soil hydraulic properties. **Vadose Zone Journal**. 16, 1–10.

Van Genuchten, M.Th., 1980. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. **Soil Science Society of America Journal**. 44, 892–897.

Van Genuchten, M. Th., Leij, F. J. Yates, S. R., 1991. the RETC code for quantifying the hydraulic functions of unsaturated soils. EPA/600/2-91/065, U.S. **Department of agriculture, agricultural Research Service Riverside**, California.

Van Genuchten, M.Th., Pachepsky, Y.A., 2011. Hydraulic Properties of Unsaturated Soils. **Image Analysis in Agrophysics** (pp.368-376).

Vereecken, H., Maes, J., Feyen, J., and Darius, P., 1989. Estimating the soil moisture retention characteristic from texture, bulk density, and carbon content. **Soil Science**. 148, 389–403.

Vereecken, H., J. Maes, and J. Feyen. 1990. Estimating unsaturated hydraulic conductivity from easily measured soil properties. **Soil Science**. 149, 1–12.

Vereecken, H., Schnepf, A., Hopmans, J.W. Javaux, M., 2016. Modeling Soil Processes: Review, Key Challenges, and New Perspectives. **Vadose Zone Journal**. 15, 1–57.

Wendroth, O., S. Koszinski, and E. Pena-Yewtukhiv. 2006. Spatial Association between Soil hydraulic properties, soil texture and geoelectrical resistivity. **Vadose Zone Journal**. 5, 341–355.

Weynants, M., Vereecken, H., Javaux, M., 2009. Revisiting Vereecken Pedotransfer Functions: Introducing a Closed-Form Hydraulic Model. **Vadose Zone Journal**. 8, 86–95.

Zhang, Y., Schaap, M.G., 2019. Estimation of saturated hydraulic conductivity with pedotransfer functions: A review. **Journal of Hydrology**. 575, 1011–1030.

Zhang, Y., Schaap, M., 2017. Weighted recalibration of the Rosetta Pedotransfer model with improved estimates of hydraulic parameter distributions and summary statistics (Rosetta3). **Journal of Hydrology**. 547, 39–53.

5 GENERAL CONCLUSIONS

Understanding the soil water behavior is essential for deciding about aspects that involve the environment at all scales. Thereby, the search for pedotransfer models that are easy to obtain and physically grounded for the analysis of soil hydraulic processes should be constant in science. This study tried to corroborate with the reduction of the risk of modelling procedures, which have been applied and extrapolated in the analysis of soils from different regions, management and conditions, from where the calibration data are originated.

The use of Splintex 2.0 model for the estimation of VGM parameters, which compose the soil water retention curve (SWRC) and hydraulic conductivity curve (SHCC), is an effective alternative based on simple key-soil variables. This result contributes with many case studies where a lack of data is present due to the high cost or difficult for the obtention of these parameters.

Furthermore, this study examined a physically-based PTF for estimating key-soil-variables for modeling SWRC and SHCC and other hydraulic functions that are derived from them, such as diffusivity, water capacity, drainable porosity, available water content, relative field capacity, and others. These variables can be considered as input parameters in hydrological and agricultural models, thus contributing for the analysis of water balance scenarios.

GENERAL REFERENCES

Arruda, F.B., Zullo, J.J., Oliveira, J.B., 1987. Soil parameters for the calculation of the available water based on soil texture. **Revista Brasileira de Ciência do Solo**. 11, 11–15.

Arya, L.M., Paris, J.F., 1981. A physico-empirical model to predict the soil moisture characteristic from particle-size distribution and bulk density data. **Soil Science Society of America Journal**. 45, 1023–1030.

Arya, L.M., Richeter, J.C., Davidson, S.A., 1982. A comparison of soil moisture characteristic predicted by the Arya-Paris model with laboratory-measured data. **Agristars Technology Resport**. Sm-L1-04247, JSC-17820, NASA-Johson Space Center, Houston, TX.

Arya, L.M., Leij, F.J., Van Genuchten, M.Th., Shouse, P.J., 1999a. Scaling Parameter to Predict the Soil Water Characteristic from Particle-Size Distribution Data. **Soil Science Society of America Journal**. 63, 510–519.

Arya, L.M., Leij, F.J., Shouse, P.J., Van Genuchten, M.Th., 1999b. Relationship between the Hydraulic Conductivity Function and the Particle-Size Distribution. **Soil Science Society of America Journal**. 63, 1063–1070.

Arya, L.M., Bowman, D.C., Thapa, B.B., Cassel, D.K., 2008. Scaling soil water characteristic of golf course and athletic field sands from particle-size distribution. **Soil Science Society of America Journal**. 72:25–32. doi:10.2136/sssaj2006.0232

Armindo, R.A., Wendroth, O., 2016. Physical soil structure evaluation based on hydraulic energy functions. **Soil Science Society of America Journal**. 80:1167–1180.

Barros, A.H.C., Van Lier, Q.J., Maia, A.H.N., Scarpare, F.V., 2013. Pedotransfer functions to estimate water retention parameters of soils in northeastern Brazil. **Revista Brasileira de Ciência do Solo**. 37, 379–391.

Bouma J., 1989. Using soil survey data for quantitative land evaluation. **Advanced Soil Science**. 9, 177–213.

Chaney, N.W., Minasny, B., Herman, J.D., Nauman, T.W., Brungard, C., Morgan, C.L.S., McBratney, A.B., Wood, E.F., Yimam, Y.T., 2019. POLARIS soil properties: 30-meter probabilistic maps of soil properties over the contiguous United States. **Water Resources Research**. 1–53.

Haghverdi, A., Öztürk, H.S., Cornelis, W.M., 2014. Revisiting the pseudo continuous pedotransfer function concept: Impact of data quality and data mining method. **Geoderma**. 227, 31–38.

Haverkamp, R.C., Zammit, F., Bouraoui, K., Rajkai, J.L.A., Heckman, N., 1997. GRIZZLY, Grenoble Soil Catalogue. Soil survey of field data and description of particle size, soil water retention and hydraulic conductivity functions. Laboratoire d'Étude des Transfers en Hydrologie et Environnement, LTHE, UMR5564, CNRS, INPG, ORSTOM, UJF, BP 53, 38041 Grenoble Cédex 09, xz France.

Hodnett, M.G., Tomasella, J., 2002. Marked differences between van Genuchten soil water-retention parameters for temperate and tropical soils: a new water-retention pedotransfer function developed for tropical soils. **Geoderma**. 108, 155–180.

McBratney, A.B., Minasny, B., Cattle, S.R., Vervoort, R.W., 2002. From pedotransfer functions to soil inference systems. **Geoderma**. 109, 41–73.

Medrado, E., Lima, J.E.F.W., 2014. Development of pedotransfer functions for estimating water retention curve for tropical soils of the Brazilian Savanna. **Geoderma Regional**. 1:59–66.

Minasny, B., McBratney, A.B., 2002. The Neuro-m method for fitting neural network parametric Pedotransfer function. **Soil Science Society of America Journal**. 66, 352–361.

Mualem, Y., 1976. A new model for predicting the hydraulic conductivity of unsaturated porous media. **Water Resource Research**. 12:513–522.

Minasny, B., McBratney, A.B., Bristow, K.L., 1999. Comparison of different approaches to the development of pedotransfer functions for water-retention curves. **Geoderma**. 93, 225–253.

Michelon, C.J., Carlesso, R., Oliveira, Z.B., Kniesi, A.E.K., Petry, M.T., Martins, J.D., 2010. Funções de pedotransferência para estimativa da retenção de água em alguns solos do Rio Grande do Sul. **Ciência Rural**. 40, 848–853.

Nemes, A., Schaap, M.G., Leij, F.J., Wosten, J.H.M., 2001. Description of the unsaturated soil hydraulic database UNSOSA version 2.0. **Journal of Hydrology**. 251, 151–162.

Oliveira, L.B., Ribeiro, M.R., Jacomine, P.K.T., Rodrigues, J.J.V., Marques, F.A., 2002. Funções de pedotransferência para predição da umidade retida a potenciais específicos em solos do estado de Pernambuco. **Revista Brasileira de Ciência do Solo**. 26, 315–323.

Ottoni, M.V., Ottoni, F.T.B., Schaap, M.G., Lopes-Assad, M.L.R.C., Rotunno, F.O.C., 2018. Hydrophysical database for Brazilian soils (HYBRAS) and pedotransfer functions for water retention. **Vadose Zone Journal**. 170095, 1–17. doi:10.2136/vzj2017.05.0095.

Pachepsky, Y.A., Rawls, W.J., 2004. Development of Pedotransfer Functions in Soil Hydrology. **In: Developments in Soil Science 30**. Elsevier, Amsterdam. 525p.

Prevedello, C.L., Loyola, J.M.T., 2002. Modelo para estimar as propriedades hidráulicas de meios porosos a partir da curva granulométrica. **Congresso Brasileiro de Mecânica dos Solos e Engenharia Geotécnica**, São Paulo, 2002. ABMS, Anais. São Paulo, pp. 467–472.

Prevedello, C.L., Maggiotto, S.R., Loyola, J.M.T., Dias, N.L. & Bepler Neto, G. 2007. Water balance for automatic data acquisition in culture of wheat (Triticum aestivum L.). **Revista Brasileira de Ciência do Solo**. 31, 1–8.

Prevedello, C.L., Armindo, R.A., 2016. Generalization of the Green-Ampt theory for horizontal infiltration into homogeneous soil. **Vadose Zone Journal**. 15, 1–10.

Reis, A.M.H., Armindo, R.A., Duraes, M.F., Lier., Q.J.V., 2018. Evaluating pedotransfer functions of the Splintex model. **European Journal of Soil Science**. 69, 685–697.

Reichert, J.M., Albuquerque, J.A., Kaiser, D.R., Reinert, D.J., Urach, F.L., Carlesso, R., 2009. Estimation of water retention and availability in soils of Rio Grande do Sul. **Revista Brasileira de Ciência do Solo**. 33, 1547–1560.

Ribeiro, K.D., Nascimento, J.M.S., Gomes N.M., Lima, L.A., Menezes, S.M., 2007. Relações matemáticas entre porosidade drenável e condutividade hidráulica do solo saturado. **Revista Brasileira de Engenharia Agrícola e Ambiental**. 11, 600–606.

Richards, L.A., Weaver, L.R., 1944. Moisture retention by some irrigated soils as related to soil moisture tension. **Journal Agricultural Research**. 69, 215–235.

Rodas, A., 1970. Determinación de la conductividad hidráulica em muestras de suelo inalterada. Lima, **CENDRET**. 118p.

Saxton, K.E., Rawls, W.J., Romberger, J.S., Papendick, R.I., 1986. Estimating generalized soil-water characteristics from texture. **Soil Science Society of America Journal**. 50, 1031–1036.

Schaap, M.G., Leij, F.J., Van Genuchten, M.Th., 2001. Rosetta: a computer program for estimating soil hydraulic parameters with hierarchical pedotransfer functions. **Journal of Hydrology**. 251, 163–176.

Scussiato, T., 2012. Study of the air flow in soils using the technique of air sparging in bidimensional physical model. **MSc thesis, Universidade de São Paulo**, Piracicaba. URL http://www.teses.usp.br/teses/disponiveis/3/3145/tde-11062013105342/en.php [accessed on 05 January 2019].

Silva, A.C., Armindo, R.A., Brito, A.S., Schaap, M.G., 2017a. Splintex: A physically-based pedotransfer function for modeling soil hydraulic functions. **Soil Tillage Research**. 174, 261–272.

Silva, A.C., Armindo, R.A., Brito, A.S., Schaap, M.G., 2017b. An assessment of pedotransfer function performance for the estimation of spatial variability of key soil hydraulic properties. **Vadose Zone Journal**. 16, 1–10.

Souza, J.L.M., Gomes, S., 2008. Limitations in the use of a ten-day water balance model, based on available water capacity in the soil. **Acta Scientiarum Agronomy**. 30, 153–163.

Soil Survey Staff., 1999. Soil Taxonomy: A Basic System of Soil Classification for Making and Interpreting Soil Surveys, Second Edition. **Natural Resources Conservation Service. U.S**. Department of Agriculture Handbook 436, Washington, DC.

Tomasella, J., Hodnett, M.G., 1998. Estimating soil water retention characteristics from limited data in Brazilian Amazonia. **Soil Science Society of America Journal**. 163, 190–202.

Tomasella, J., Hodnett, M.G., Rossato., L., 2000. Pedotransfer functions for the estimation of soil water retention in Brazilian soils. **Soil Science Society of America Journal**. 64, 327–338.

Tomasella, J., Hodnett, M.G., Cuartas, L.A., Nobre, A.D., Waterloo, M.J., Oliveira, S.M., 2008. The water balance of an Amazonian micro-catchment: the effect of interannual variability of rainfall on hydrological behaviour. **Hydrological Processes**. 22, 2133–2147.

Turek, M.E., Armindo, R.A., Wendroth, O., Santos, I., 2018. Criteria for the estimation of field capacity and their implications for the bucket type model. **European Journal Soil Science**. 69, 1–8.

USDA-NRCS., 1997. National Soil Characterization Database. **USDA-NRCS Soil Survey Division**. http://www.statlab.iastate.edu/soils/ssl/natch_data.html.

Van Genuchten, M.Th., 1980. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. **Soil Science Society of America Journal**. 44, 892–897.

Van Lier, Q.J., Wendroth, O., Van Dam, J., 2015. Prediction of winter wheat yield with the SWAP model using pedotransfer functions: An evaluation of sensitivity, parameterization and prediction accuracy. **Agricultural Water Management on Science Direct**. 154, 29–42.

Van Lier, Q.J., 2017. Field capacity, a valid upper limit of crop available water. **Agricultural Water Management on Science Direct**. 193, 214–220.

Van Looy, K., Bouma, J., Herbst, M., Koestel, J., Minasny, B., Mishra, U., Vereecken, H., 2017. Pedotransfer functions in Earth system science: Challenges and perspectives. **Reviews of Geophysics**. 55, 1199–1256. https://doi. org/10.1002/2017RG000581.

Vaz, C.M.P., Iossi, M.F., Naime, J.M., Macedo, A., Reichert, J.M., Reinert, D.J. et al. 2005. Validation of the Arya and Paris water retention model for Brazilian soils. **Soil Science Society of America Journal**. 69, 577–583.

Vereecken, H., Feyen, J., Maes, J., 1989. Estimating the soil moisture retention characteristic from particle size distribution, bulk density and carbon content. **Soil Science**. 148, 389–403.

Wösten, J.H.M., Van Genuchten, M.Th., 1988. Using Texture and Other Soil Properties to Predict the Unsaturated Soil Hydraulic Functions. **Soil Science Society of America Journal**. 52, 1762–1770.

Wösten, J.H.M., Pachepsky, Ya.A., Rawls, W.J., 2001. Pedotransfer functions: bridging the gap between available basic soil data and missing soil hydraulic characteristics. **Journal of Hydrology**. 251, 126–150.

Zhang, Y., Schaap, M.G., Guadagnini, A., Neuman, S.P., 2016. Inverse modeling of unsaturated flow using clusters of soil texture and Pedotransfer functions. **Water Resources Research**. 52, 1–14.

Zhang, Y., Schaap, M., 2017. Weighted recalibration of the Rosetta Pedotransfer model with improved estimates of hydraulic parameter distributions and summary statistics (Rosetta3). **Journal of Hydrology**. 547, 39–53.

APPENDIX - REGISTRATION CERTIFICATE OF THE COMPUTER PROGRAM: SPLINTEX

REPÚBLICA FEDERATIVA DO BRASIL
MINISTÉRIO DA INDÚSTRIA, COMÉRCIO EXTERIOR E SERVIÇOS
INSTITUTO NACIONAL DA PROPRIEDADE INDUSTRIAL
DIRETORIA DE PATENTES, PROGRAMAS DE COMPUTADOR E TOPOGRAFIAS DE CIRCUITOS INTEGRADOS

Certificado de Registro de Programa de Computador

Processo Nº: **BR512018001393-7**

O Instituto Nacional da Propriedade Industrial expede o presente certificado de registro de programa de computador, válido por 50 anos a partir de 1° de janeiro subsequente à data de 17/07/2018, em conformidade com o §2°, art. 2° da Lei 9.609, de 19 de Fevereiro de 1998.

Título: Splintex - Modelo de Pedotransferência

Data de criação: 17/07/2018

Titular(es): UNIVERSIDADE FEDERAL DO PARANA

Autor(es): ROBSON ANDRÉ ARMINDO; ALESSANDRA CALEGARI DA SILVA; CELSO LUIZ PREVEDELLO

Linguagem: C++

Campo de aplicação: AG-06; AG-07; CC-09; MA-03; MA-04; PD-02

Tipo de programa: FA-01; GI-01; SM-01

Algoritmo hash: SHA-512

Resumo digital hash:
5E08B720E61459DA45749F7AE2BA65D18C31243A4F938160BF0F41BAC50B3103DA15414DC2C6CD7F1928BFC9
1E8783AB0EB265504839120F5533E9221AD377A2

Expedido em: 14/08/2018

REPÚBLICA FEDERATIVA DO BRASIL
15 de Novembro de 1889

Aprovado por:
Liane Elizabeth Caldeira Lage
Diretora de Patentes, Programas de Computador e Topografias de Circuitos