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SPLINTEX: A physically-based pedotransfer function for modeling soil hydraulic functions

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ABSTRACT

The determination of soil hydraulic properties is laborious and expensive, especially in large-scale applications. One often used substitute for measured hydraulic properties are pedotransfer function (PTFs) estimates. Most PTFs, however, are statistical models that tend to produce biased results for data outside their –often limited– calibration databases. In addition, most PTFs have been established on data derived from temperate regions causing the question whether such models are applicable to soils in tropical regions. This work aimed to evaluate the performance of the *Splintex* PTF to predict the hydraulic functions for sandy and clayey soils from several tropical and subtropical Brazilian datasets. *Splintex* is somewhat unique in that it is based on physical principles using a modification of the Arya-Paris method while allowing the estimation of van Genuchten parameters from limited data. In addition, *Splintex* has an option to include measured soil water retention points, in principle allowing it to produce accurate estimates for a variety of soils. Estimates by *Splintex* were compared with the empirical *Rosetta* PTF, which also has an option to use one (or two) retention points. Estimates by both PTFs were compared to observed retention data and field capacity, available water capacity, hydraulic conductivity, and diffusivity using metrics such as Pearson correlation (r), mean absolute error (MAE) and root mean square error (RMSE). Both *Splintex* and *Rosetta* yielded similar results and sometimes produced significant biases in estimated quantities. In the majority of cases it appears that *Splintex* produced somewhat better estimates than the 2001 version of *Rosetta*, indicating that *Splintex* is a viable, physically-based, alternative to estimating hydraulic properties.

1. Introduction

Knowledge about water dynamics in the soil-plant-atmosphere system has increased significantly over the past decades. One crucial area where only limited advances have been made is that of the quantification of soil hydraulic properties, which play an important role in crop production, irrigation, infiltration and drainage, water stress, evapotranspiration as well as in heat, gas and solute transport. Especially at large scales it is often difficult to obtain reliable data about the soil water retention curve (SWRC) and unsaturated hydraulic conductivity [K(θ)], both of which are needed for the modeling of soil water dynamics with the Richards equation.

Pedotransfer functions (PTFs) offer an indirect alternative to estimate soil hydraulic properties (Bouma, 1989). In general, PTFs can be defined as methods that predict soil variables that are difficult to measure using correlations with soil attributes that are widely available or can be determined cheaply. Several studies (e.g., McBratney et al., 2002; Botula et al., 2014; Haghverdi et al., 2014) have developed PTFs for estimating SWRC making use of a range of statistical techniques, which relate physical and chemical soil properties [typically texture, bulk density (ρ_b) and organic matter (OM)] with parameters that characterize the SWRC.

Most published PTFs have been developed using datasets collected in temperate climates. PTFs developed specifically for tropical soils are comparatively rare, with most work conducted for Brazilian soils and their data sets. For example, Tomasella and Hodnett (1998) developed PTFs for selected soils from the tropical Amazon region. PTFs for temperate southern Brazil were developed by Reichert et al. (2009) and Michelon et al. (2010) while Oliveira et al. (2002) established PTFs for hot and semi-arid parts of Eastern Brazil. In addition, Barros et al. (2013) developed PTFs to carry out simulations of agricultural crop yield for northeastern Brazil using the hydrological model Soil Water

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Atmosphere Plant (SWAP) (van Dam et al., 1997). PTFs for several Brazilian states were developed by Tomasella et al. (2000), Hodnett and Tomasella (2002), and Tomasella et al. (2003), while Fidalski and Tormena (2007) and Silva et al. (2008) developed PTFs that not only predicted SWRC but also soil penetration resistance curve (SPRC).

All available PTFs suitable for tropical soils are based on regression techniques using databases of limited size. As input these PTFs typically use only textural classes and do not incorporate information about soil structure, which directly influences the hydraulic behavior (Weynants et al., 2009). In addition, these authors criticize their wide use in geographic regions that are different from those that they were developed, generally with different geology, hydrogeology, climate, and soil use.

An alternative to overcoming the empiricism inherent in statistical methods is the development of PTFs based on physical considerations. This can be accomplished using physical equations that link soil texture to hydraulic properties. Prevedello and Loyola (2002) developed the *Splintex* PTF, which is a modification of the physico-empirical Arya and Paris (1981) model. Instead of requiring detailed particle size distributions, *Splintex* uses limited texture data that are fitted with the cubic spline function. The model is able to provide its output in the form of van Genuchten (1980) parameters. In addition, *Splintex* offers the possibility to include saturated water content as well as a measured water retention point at arbitrary pressure head into its predictors. Even though the estimation of soil water retention is the *objective* of many PTFs it has been demonstrated by Rawls et al. (1992) and Schaap et al. (1998) that the inclusion of one or more measured retention points can significantly improve the estimation of hydraulic parameters. In effect, including a retention point into the set of predictors allows the PTF to adjust for soil-specific variations that may otherwise be very hard to identify or quantify.

Even though the *Splintex* PTF has been used in several publications (Prevedello et al., 2007; Souza Filho and Gomes, 2007; Souza and Gomes, 2008; Souza et al., 2015) its performance has never been formally assessed. This study is therefore aimed to evaluate the performance of *Splintex* to predict the soil hydraulic functions of several sandy and clayey Brazilian soils. Its performance is compared with the empirical *Rosetta* PTF. *Rosetta* was specifically chosen for this study because, similar to *Splintex*, it also allows one or two water retention points to be used to estimate van Genuchten (1980) parameters. Very few other PTFs allow the inclusion of retention points and it is interesting to investigate whether a physically-based performs better than a purely data-driven approach.

In the following precision and accuracy of estimates by *Splintex* and *Rosetta* for both the SWRC as well as unsaturated hydraulic conductivity will be compared. To this end we will first describe the soil data collected, and briefly introduce *Splintex* and *Rosetta*, as well as the evaluation metrics used. The evaluation will be carried out on the basis of van Genuchten (1980) parameters, which are the primary outputs of both *Splintex* and *Rosetta*. However, we will also evaluate the accuracy of field capacity, water capacity, and diffusivity. The derived properties have a physical or conceptual interpretation and often play important roles in predictions of water uptake by plants and are also related to the evaporation and infiltration of water into the soil (Conceição et al., 2014).

2. Material and methods

The data set used was composed of 60 undisturbed cores collected between 0.75 and 0.85 m depth in a sandy soil under a fallow area from Piracicaba city, São Paulo state, Brazil (Brito et al., 2011). In addition 43 samples were included from the literature (Barcelos, 1996; Aguiar, 2008; Nunes, 2006; Silva et al., 2006; Uhde, 2009; Lucas, 2010; Gimenes, 2012; Souza, 2012; Oliveira, 2014). These soil data sets are from several Brazilian regions and sampled at depths between 0.20 and 0.30 m. The SWRC, bulk density (ρ_b), particle density (ρ_p) and the particle size distribution considering the particle diameter d of sand ($0.05 \leq d < 2$ mm), silt (0.05 mm $< d \leq 0.002$ mm) and clay ($d < 0.002$ mm) were available for each of the 103 samples.

The SWRC was determined in the laboratory (for the sandy soil) with undisturbed core samples using the hanging water column method (Dane and Hopmans, 2002a) at soil water matric tensions of 10, 20, 30, 40, 50, 60, 70, 80, 90, and 100 hPa. The samples were then taken to a pressure plate apparatus where water retention points at 300, 500, 700, and 1000 hPa were obtained (Dane and Hopmans, 2002b). The van Genuchten (1980) equation was fitted to each of the SWRCs:

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

in which $\theta(h)$ is the volumetric water content ($m^3\,m^{-3}$) as a function of the soil water matric tension (h), with $h > 0$ for unsaturated conditions. The parameters θ_s and θ_r are saturated and residual water contents ($m^3\,m^{-3}$), respectively; α (hPa^{-1}) and n are empirical curve shape factors. The saturated soil water content (θ_s) was set to the soil total porosity value (ϕ), as accomplished by Medrado and Lima (2014).

After fitting the van Genuchten (1980) parameters for all of the 103 SWRCs, four soil water content (θ) values were generated using the soil water tension (h) values at 30, 60, 100, and 330 hPa for feeding *Splintex* and *Rosetta*.

Saturated hydraulic conductivity (K_s) was measured for the sixty sandy samples (the Piracicaba city data) according to the Libardi et al. (1980) method. No such data were available for the 43 clay soil samples.

The values of ρ_b were determined using undisturbed samples with volumetric rings (Blake and Hartge, 2002). Disturbed samples were used (for the sandy soil) for determining ρ_p using the gas pycnometer (Flint and Flint, 2002) and texture using 2 mm diameter sieves and then pipette method (Gee and Or, 2002).

2.1. Estimation of SWRC parameters using Splintex and Rosetta

Splintex (Prevedello and Loyola, 2002) is a semi-physical model based on the Arya and Paris (1981) model (AP). Similar to the Arya-Paris model, *Splintex* assumes that the SWRC has a curve-shape similarity with the cumulative particle size distribution (PSD), and in addition it is based on the assumption that PSD can be described with a spline function (Prevedello and Loyola, 2002). This greatly improves the applicability of the AP approach because it allows an arbitrary number (N) of texture fractions to be evaluated by interpolation and allows the use of as few as three measured texture fractions (e.g. sand, silt, and clay).

Similar to Arya and Paris (1981) and Arya et al. (1999), *Splintex* predicts points on the SWRC (h_i, θ_i) using the soil-water capillary equation to predict soil water matric tension:

$$h_i = 2\sigma/(\rho_w\, g\, r_i) \quad (2)$$

and the weight fraction of a texture range to compute soil water content:

$$\theta_i = \phi \Sigma w_i \quad (3)$$

Subscript i denotes the i^{th} texture class; σ is the surface tension of the air-water interface, ρ_w is the density of water, g is the acceleration of gravity, ϕ is the soil porosity. The key feature in the Arya-Paris model is the relation between the i^{th} pore radius (r_i), and the i^{th} soil mass fraction (w_i) as well as the i^{th} soil particle radius (R_i) which are combined considering a spherical particle packing and the scaling factor (α_{AP}) (Arya and Paris, 1981; Arya et al., 1999).

Splintex has several options by which it can generate van Genuchten (1980) parameters. In its most basic version, it simply estimates pairs of (θ_i, h_i) after which it obtains the VG parameters by curve fitting. Several publications, however, have demonstrated that α_{AP} varies for different soils. In order to correct the estimation deviations, two measured θ