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Using splines in the application of the instantaneous profile method for the hydrodynamic characterization of a tropical agricultural Vertisol

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ABSTRACT: An important aspect in the study and understanding of the physical phenomena involved in water movement in the soil-plant system is the need to carry out the hydrodynamic characterization (HC) of non-saturated field soils. Studies of this type have been widely developed in soils of temperate climates, but they are infrequent in the tropics, hence there is a need for further research in tropical Vertisols under field conditions. Hydrodynamic characterization consists of finding the functional relationship between soil hydraulic conductivity (*K*), matric head (*h*) and soil moisture content (θ), widely known as $K(\theta)$ and $h(\theta)$ relationships, being the main objective of this study. The instantaneous profile method (IPM) was applied, in which splines were used for the HC of a bare, tropical agricultural field soil classified as a Vertisol. Field measurements of *h* and θ were made at five different soil depths (0.15, 0.30, 0.45, 0.60 and 0.90 m) and values of *K* at the same depths were estimated with the IPM, which allowed for the estimation of pairs of values of the $K(\theta)$ relationships in the soil profile. Unlike in other studies with the same objective, the use of splines was proposed to represent the spatial variation of the *H(z)* and $\theta(z)$ functions in the IPM. Subsequently, the van Genuchten equation was adjusted to the specific values determined for the $h(\theta)$ relations (r^2 value ranged from 0.65 to 0.87), and the *Ks* values and the point data of *K* and θ were used to estimate the accuracy of the equation proposed by Mualem–van Genuchten (M-vG): in this case negative values for the exponent *l* of the M-vG function were determined for the five soil depths under study, ranging from –7.04 (0.45 m deep), to -13.26 (0.90 m deep). In addition, pedotransfer functions for tropical soils proposed in the literature, based on different soil physical properties, were used to estimate the $h(\theta)$ and $K(\theta)$ relationships and the saturated hydraulic conductivity (*Ks*). Best square root of the mean squared error (SRMSEθ) observed was 0.02853 $cm^3\ cm^{-3}$ at 0.15 m depth and 0.02262 $cm^3\ cm^{-3}$ at 0.9 m depth for $h(\theta)$ relations, and in all cases, the SRMSE*k* values are less than 0.0018 m day^{-1} for $K(\theta)$ relationships. The results reveal the utility of splines in the IPM for characterizing the soil profile $K(\theta)$ relationships in field studies, as well as the need for more research to the generation of pedotransfer functions in tropical Vertisols.

Keywords: Calcic Vertisol, unsaturated field soil, hydraulic conductivity, Mualem–van Genuchten equation, pedotransfer functions.

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INTRODUCTION

Vertisols occupy 9.5 million hectares in Mexico, which correspond to 8.3 % of the national territory (INEGI, 2014). There is a dearth of information on hydrologic processes to improve agronomic practices on Vertisols (Torres-Guerrero et al., 2016). Soil hydrodynamic properties, represented by the relationships between soil water matric head (h), soil hydraulic conductivity (K), and volumetric soil moisture content (θ), widely known as the $h(\theta)$ and $K(\theta)$ functions, are of great importance in many scientific fields, such as hydrology, environmental sciences and agronomy (Peña-Sancho et al., 2017). Vertisols shrink to form deep vertical cracks in the dry state, producing macropores, and upon rewetting, the soil swells due to the presence of expanding clay minerals (Favre et al., 1997; Dinka and Lascano, 2012), complicating its hydrodynamic characterization (HC). This Vertisols property makes it necessary to carry out their HC under field conditions, as was done in the present study, because otherwise, it is very difficult to consider the effects of macroporosity.

In hydrology, knowledge of both functions is essential for practical reasons, such as modeling the movement of water and solutes in unsaturated soils (Kool and van Genuchten, 1991; Šimůnek and van Genuchten, 1994; Šimůnek et al., 2012; Ahmadi et al., 2015). Ecologists use $h(\theta)$ and $K(\theta)$ relations to calculate the ecosystems maintenance, such as wetlands (Eldridge and Freudenberger, 2005; Colloff et al., 2010), and also in studies dealing with groundwater quality and pollution, both point and diffuse, the storage of waste, the decontamination of aquifers, among others (Donado-Garzón, 2004).

In agronomy, soil $K(\theta)$ relationships play an important role in determining the rate at which soil water enters the root system and thus play a decisive role in determining crop yield (Wetzel and Chang, 1987; Zhang et al., 2004). Crop yield has also been shown to be highly dependent on the value of soil water matric head h, used as an indicator of the onset of irrigation in different crops, such as potatoes (*Solanum tuberosum*) (Kang et al., 2004; Wang et al., 2007; Carli et al., 2014), bananas (*Musa AAA*) (Orozco-Romero and Pérez-Zamora, 2006), sweet corn (*Zea mays*) (Rivera-Hernández et al., 2009, 2010), rice (*Oryza sativa*) (Sudhir-Yadav et al., 2011; Mahajan et al., 2012), sunflowers (*Helianthus annuus*) (Carrillo-Ávila et al., 2015), sugar cane (*Saccharum officinarum*) (Alamilla-Magaña et al., 2016) and habanero peppers (*Capsicum chinense* Jacq) (Gutiérrez-Gómez et al., 2018), among others.

In contrast, the application of irrigation water affects a wide variety of water transfer processes, such as surface runoff, infiltration and water loss below the root zone (Bachmann et al., 2006), whose magnitude depends fundamentally on soil $h(\theta)$ and $K(\theta)$ relationships, that must therefore be precisely determined in order to quantitatively analyze these processes (Villagra et al., 1994).

There are different methods for estimating soil $h(\theta)$ and $K(\theta)$ relationships, whether direct, by using measurements of h, θ and K under laboratory or field conditions, or by applying pedotransfer functions (PTFs) in which the relationships are estimated from other soil physical properties, such as bulk density, texture and organic carbon content, among others. Lu and Likos (2004) stated that soil properties, such as pore-size distribution, particle-size distribution, mineralogy, bulk density and organic matter content, among others, strongly influence the shape of the $h(\theta)$ curve. However, the vast majority of PTFs have been developed for temperate regions (Campbell and Campbell, 1982; Puckett et al., 1985; Vereecken et al., 1989; Ogilvi, 1990; Wösten et al., 1999; Slater and Lesmes, 2002; Rajkai et al., 2004; Shevnin et al., 2006; Peinado-Guevara et al., 2010; Delgado-Rodríguez et al., 2011; Patil and Singh, 2016). For tropical soils, Minasny and Hartemink (2011) reviewed PTFs proposed in the literature. In the case of tropical soils, very little research has been conducted to date. Vertisols are known for their pronounced macroporous structure in an almost impermeable matrix (clay). Most PTFs do not consider macropores, and those that do have had great difficulty simulating

the behavior of the preferential flow of water that occurs through macropores. Some attempts have been made to perform hydrodynamic characterization in macroporosity soils, and have mainly focused on the estimation of hydraulic conductivity and solute transport (Luo et al., 2010; Zhang et al., 2019). To our knowledge, only the researchs of van den Berg et al. (1997), Tomasella and Hodnett (1998), Hodnett and Tomasella (2002), Tomasella et al. (2000) and Tomasella et al. (2003), proposed PTFs for the $h(\theta)$ relation, while Tomasella and Hodnett (1997) and Agyare et al. (2007) proposed PTFs for the estimation of the $K(\theta)$ relationship and saturated hydraulic conductivity in tropical soils.

This study presents results of the field characterization of the $h(\theta)$ and $K(\theta)$ relationships in a bare, tropical, agricultural Vertisol with pronounced secondary structure and a water table present near the surface. To estimate the $K(\theta)$ relationship, K values for different soil water contents θ were determined by applying the instantaneous profile method (Watson, 1966; Cheng et al., 1975; Vachaud et al., 1981; Vauclin and Vachaud, 1987; Mohanty and Singh, 1996; Leung et al., 2016) under field conditions, in the case where a zero flux plane is present in the soil profile. When applying the method, for reasons of simplicity and unlike other studies carried out with the same objective, this study uses splines to express the variation of the total head H and volumetric soil water content with depth z ($H(z)$ and θ (z)). To the best of our knowledge, there is no other study in the scientific literature in which splines have been used in the instantaneous profile method, in order to perform the hydrodynamic characterization of a tropical Vertisol under field conditions. Splines are a set of curves that connect points crossing them exactly and forming continuous curves. There are different types of splines depending on the functional relationship used to join the points. As McClarren (2018) explained, a cubic spline is a piecewise cubic function that interpolates a set of data points and provides smoothness across all data points. Between each pair of points, cubic functions are used to interpolate among the values. In addition, the first and second derivatives of the functions used to construct splines must be continuous, in order to ensure that the points are joined as smoothly as possible with their neighbors (Siauw and Bayen, 2015).

Until now, few studies to determine the $h(\theta)$ and $K(\theta)$ relationships in tropical soils and under field conditions has been developed, most of the hydrodynamic characterization studies having been carried out in soils of temperate climates (Botula et al., 2012). This study aimed to perform the hydrodynamic characterization of a tropical Vertisol at field conditions, under the hypothesis that the instantaneous profile method, in which splines were used to express the variation of the total head and of the volumetric soil water content with depth, can be applied in tropical Vertisol soils, to determine the $K(\theta)$ relationships at different soil profile depths. Pedotransfer functions for tropical soils proposed in the literature, based on different soil physical properties, were used to estimate the $h(\theta)$ and $K(\theta)$ relationships and the saturated hydraulic conductivity (Ks), and the results obtained in the two methods were compared.

MATERIALS AND METHODS

Study area and soil physical characteristics

The study was carried out on a tropical, agricultural, bare soil, classified as calcium Vertisol according to the Food and Agriculture Organization of the United Nations (FAO) classification (Rivera-Hernández et al., 2010), located in the Champotón municipality, Campeche State, Mexico (19° 29’ 54” N; 90° 32’ 54” W and 20 m a.s.l.), with the presence of a water table at about 1 m deep. The predominant climate in the state of Campeche is warm sub-humid, with rainfall during summer, classified as AW_0 according to Köppen climatic classification modified by García (1973). Average annual temperature is 26.8 °C, with the highest monthly average temperature in May (29.6 °C) and the lowest in January

(23.2 °C). Average annual rainfall is 1099 mm. Between June and November, during the rainy season, frequent and high-intensity rainfall occurs. In contrast, February to May is the dry/drought season, a period having the lowest rainfall and highest temperatures (Gutiérrez-Gómez et al., 2018).

Five soil depths intervals were studied (0.00-0.15, 0.15-0.30, 0.30-0.45, 045-0.60 and 0.60-0.90 m), whose main physical properties are summarized in table 1. Soil bulk density determination was carried out with an Uhland type auger, soil organic matter content with the method proposed by Walkley-Black (Hernán et al., 2013; Bahadori and Tofighi, 2017) and soil texture with the Bouyoucos hydrometer method, at the five soil depths intervals. Soil organic matter content and texture determinations were performed on a composite soil sample. Soil texture classification was based on the United States Department of Agriculture's (USDA) particle-size distribution, with the clay fraction <2 µm, silt fraction 2–50 µm and sand fraction 50–2,000 µm. Mean soil profile values for cation exchange capacity and pH were 38 $cmol_c\ kg^{-1}$ and 6.53, respectively; they were determined on a composite soil sample.

Study period

The hydrodynamic characterization of the soil profile was carried out from May 3 to 18, 2018 in the drought season, a period during which no rain was recorded. A zero flux plane of water near the soil surface was induced by applying water to the soil surface and monitoring its redistribution in the soil profile, in a similar way described by Vachaud et al. (1981). Consequently, on May 3, water was applied to the soil surface, after which the spatial and temporal distributions of h and θ in the soil profile were measured. A near-surface water table was observed and the groundwater depth was measured in an observation well with a graduated transparent plastic hose. The depth of the water table was approximately one meter deep during the study period, increasing the value of the total head H near the bottom of the soil profile, H being the sum of matric head, pressure head, gravitational head, osmotic head and pneumatic head.

Soil water content (θ) and soil water matric head (h) measurement

After the application of water to the soil surface, the volumetric moisture content (θ) of the soil profile was measured twice daily, at 7:00 am and 6:30 pm (UTC -5), and at five depths (0.15, 0.30, 0.45, 0.60 and 0.90 m) using a time domain reflectometry (TDR) probe (IMKO, TRIME-IPH PICO-BT model), as described by Topp and Davis (1985). For the determination of the soil volumetric moisture content at different profile depths, an access tube (polyvinyl chloride –PVC-, 0.05 m in diameter) was installed to a depth of 1.4 m using a Dutch Edelman auger, similarly to Nyakudya et al. (2014) and Wiyo et al. (2000). The TDR probe was previously calibrated for each depth (Rivera-Hernández et al., 2018) to verify accuracy. The coefficient of determination (r^2) obtained between the values

Table 1. Soil physical properties, soil organic matter content (OM) and texture determinations performed on a composite soil sample

Layer	ρ	OM	Clay	Silt	Sand
m	$Mg\ m^{-3}$	%		$g\ kg^{-1}$	
0.00–0.15	1.05	2.3	780	100	120
0.10–0.30	1.09	1.6	800	100	100
0.30–0.45	1.04	1.6	840	40	120
0.45–0.60	1.07	1.4	820	40	140
0.60–0.90	1.17	1.0	800	60	140

ρ: bulk density; OM: soil organic matter content.

measured with the probe and those determined gravimetrically ($r^2 = 0.83$, $p < 0.001$) was greater than the values obtained in similar a study conducted by Wiyo et al. (2000) and Nyakudya et al. (2014) ($r^2 = 0.69$ and $r^2 = 0.72$, respectively) and was, therefore, considered acceptable. Five replications were conducted with the TDR probe and averaged for each profile depth to reduce measurement errors.

The soil water matric head *h* was measured simultaneously with the soil moisture content measurement, using pressure gauge tensiometers (Irrometer©, model "R") installed at the same depths as the soil volumetric water content measurements. The tensiometers were calibrated with a manual suction pump (Migliaccio et al., 2015) and their field installation was performed in a similar manner to that described by Rivera-Hernández et al. (2010), Alamilla-Magaña et al. (2016) and Gutiérrez-Gómez et al. (2018).

h(*θ*) relationships

To establish the *h(θ)* relationship at each soil depth, the equation proposed by van Genuchten (1980) was adjusted to the pairs of values of *h* and *θ* for each depth in the soil profile:

$$\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{[1+(\alpha h)^n]^m} \quad \text{Eq. 1}$$

$$m = 1 - 1/n \quad \text{Eq. 2}$$

In which: *θ* is the volumetric soil water content ($cm^3\,cm^{-3}$); *θr* is the volumetric residual water content ($cm^3\,cm^{-3}$); *θs* is the saturated volumetric water content ($cm^3\,cm^{-3}$); *h* is the soil water matric head (cm); *α* is a model parameter (cm^{-1}); *n* and *m* are the Shape parameters (dimensionless).

The parameter *θs* was estimated based on the particle and bulk densities (the latter being determined at each point-measurement depth), being considered numerically equal to the soil porosity, and calculated based on the mass-volume relationships of the soil. The other parameters in equation 1 were adjusted using a non-linear regression technique according to the Levenberg–Marquardt algorithm (Marquardt, 1963) by minimizing the sum of the squares of the differences between the soil water content values observed and those estimated. The differences between the measured and fitted values were assumed to follow a normal distribution. The Levenberg–Marquardt algorithm combines the Gauss–Newton and gradient-descent methods to locate the minimum in the optimized objective function. The coefficient of determination r^2 and the square root of the mean squared error (SRMSE*θ*) between the measured and fitted values of *θ* was calculated at each point-measurement depth according to equation 3.

$$SRMSE\theta = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(\theta_m - \theta_f)^2} \quad \text{Eq. 3}$$

In which: θ_m was the measured volumetric soil water content; θ_f was the fitted volumetric soil water content; and n was the number of data points used.

K(*θ*) relationships

To determine point values of the *K*(*θ*) relationships, the instantaneous profile method (Watson, 1966; Cheng et al., 1975; Vachaud et al., 1981; Vauclin and Vachaud, 1987; Mohanty and Singh, 1996; Leung et al., 2016) was applied under field conditions, when a zero-water-flux condition was observed in the soil profile, similar to Vachaud et al. (1981). The theoretical basis is reproduced in the following lines, with the sole purpose of establishing the procedure used in this study.

Theory

One-dimensional water flow

Assuming an insignificant role for the air phase in the process, the one-dimensional vertical flow of water in a rigid, porous soil without vegetation and partially saturated with water is determined by the following equations (Richards, 1931; Vauclin and Vachaud, 1987):

$$\frac{\partial q(z,t)}{\partial z} = - \frac{\partial \theta(z,t)}{\partial t} \quad \text{Eq. 4}$$

$$q(z,t) = -K(\theta) \frac{dH}{dz} \quad \text{Eq. 5}$$

Equation 4 is known as the mass conservation equation, and equation 5 is the generalized Darcy's law for unsaturated soils, where $q(z,t)$ is the vertical water flow rate (cm s^{-1}), z is the vertical axis assumed positive downward in the soil profile (cm), θ (z, t) is the volumetric soil water content (cm^3 cm^{-3}), t is the time (s), $K(\theta)$ is the hydraulic soil conductivity (cm s^{-1}), and $H(z, t)$ is the total head within the soil profile (cm).

Assuming that the pneumatic and osmotic potentials are negligible, the total head (H) in the soil includes the gravitational head (z) plus the matric head (h), as follows (Vauclin and Vachaud, 1987):

$$H = h(\theta) - z \quad \text{Eq. 6}$$

From equation 4, this gives:

$$\partial q = - \frac{\partial \theta}{\partial t} \partial z \quad \text{Eq. 7}$$

By integrating equation 7 from depth z_1 to depth z_2, gives:

$$q(z_2) - q(z_1) = - \frac{\partial}{\partial t} \int_{z_1}^{z_2} \theta(z,t) dz \quad \text{Eq. 8}$$

from which:

$$-q(z_1) = -q(z_2) = - \frac{\partial}{\partial t} \int_{z_1}^{z_2} \theta(z,t) dz \quad \text{Eq. 9}$$

By substituting equation 5 into equation 9, gives:

$$K(\theta) \frac{dH}{dz}\Big]_{z_1} = K(\theta) \frac{dH}{dz}\Big]_{z_2} - \frac{\partial}{\partial t} \int_{z_1}^{z_2} \theta(z,t) dz \quad \text{Eq. 10}$$

If, within the soil profile, the water flux is zero at a given point z_2, due to the presence of a null hydraulic gradient dH/dz at this point, which generally appears after considerable water supply at the soil surface followed by prolonged drought, the first term to the right of the equals sign in equation 10 is equal to zero, so that the equation becomes:

$$K(\theta) \frac{dH}{dz}\Big]_{z_1} = - \frac{\partial}{\partial t} \int_{z_1}^{z_2} \theta(z,t) dz \quad \text{Eq. 11}$$

from which the hydraulic conductivity is obtained as:

$$K(\theta)]_{z_1} = \frac{- \frac{\partial}{\partial t} \int_{z_1}^{z_2} \theta(z,t) dz}{\frac{dH}{dz}\Big]_{z_1}} \quad \text{Eq. 12}$$

Using equation 12, the K value was estimated at depth z_1 where the soil moisture content was also measured, for the days during which a zero flux occurred at a given point of the soil profile (ie., at depth z_2). With the h values measured within the soil profile, equation 6 allows the estimation of H at different depths, as well as the estimation of the dH/dz gradient within the soil profile. Finally, the numerator in equation 12 was estimated with:

$$\frac{\partial}{\partial t}\int_{z_1}^{z_2}\theta(z,t)dz \approx \frac{\left[\int_{z_1}^{z_2}\theta(z,t)dz\right]_{(t)} - \left[\int_{z_1}^{z_2}\theta(z,t)dz\right]_{(t-1)}}{\Delta t} \quad \text{Eq. 13}$$

Where t is the time of day when equation 13 was evaluated (hours), t - 1 is the measurement time from θ previous to t (hours), $\Delta t = t$ - (t-1), z_1 is the depth analyzed to determine K (cm), and z_2 is the depth of zero water flux (cm).

Here, unlike in other studies conducted with the same objective (Watson, 1966; Cheng et al., 1975; Vachaud et al., 1981; Vauclin and Vachaud, 1987; Mohanty and Singh, 1996; Leung et al., 2016), cubic splines were adjusted to the $H(z)$ and $\theta(z)$ data measured at different depths of the profile (z). Cubic splines were used because they fit the data perfectly and because the integration and derivation of the third-degree-polynomial equations that make up the splines are easily evaluated. Third-degree-polynomial equations integration and derivation were used later to evaluate equations 12 and 13 to estimate the point values of K at different soil depths z_1 (0.15, 0.30, 0.45, 0.60 and 0.90 m). For days when K values were estimated, h and θ values were also determined at the same depths; thus pairs of $K(h)$ and $K(\theta)$ relationship values for the five depths of the profile were available.

In contrast, values of the saturated hydraulic conductivity Ks were determined in the soil profile with the double-cylinder method (Fatehnia and Tawfiq, 2014). Later, the values of Ks and the point data of K and θ of the five soil depths under study were used to verify the accuracy of the equation proposed by Mualem–van Genuchten (van Genuchten, 1980; Schaap and van Genuchten, 2006) for $K(\theta)$:

$$K(\theta) = K_s S_e^l [1-(1 - S_e^{1/m})^m]^2 \quad \text{Eq. 14}$$

in which m is the parameter in equation 1; l is an empirical pore-connectivity parameter, currently fixed at a value of 0.5 (Mualem, 1976; Schaap and van Genuchten, 2006), and:

$$Se = \frac{\theta - \theta_r}{\theta_s - \theta_r} \quad \text{Eq. 15}$$

The value of parameter l was first set equal to 0.5 (theoretical value) to check its validity, but later, the l value was determined by fitting equation 14 to the point data of K and θ at the five soil depths. In both cases, the SRMSEk between the measured and fitted K values was calculated at all the soil profile depths (Equation 16), similarly than for θ values:

$$SRMSEk = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(K_m - K_f)^2} \quad \text{Eq. 16}$$

In which K_m is the soil hydraulic conductivity measured, K_f is soil hydraulic conductivity fitted, and n was the number of data points used.

Comparison of $h(\theta)$ and $K(\theta)$ estimates from tropical pedotransfer equations

Once the hydrodynamic functions, $h(\theta)$ and $K(\theta)$, of the soil profile were characterized, the accuracy of several literature proposed pedotransfer functions for tropical soils were tested. Minasny and Hartemink (2011) pointed out that much less research concerning pedotransfer functions has been conducted on tropical soils than in soils in temperate

climates (Hartemink, 2002), because in tropical countries there are many more limitations in budget and equipment for conducting soil-based research (Bekunda, 2006). Pedotransfer equations estimate the $h(\theta)$ and $K(\theta)$ functions or Ks as a function of soil physical properties. For the estimation of the $h(\theta)$ relationships, pedotransfer equations proposed for tropical soils by van den Berg et al. (1997), Hodnett and Tomasella (2002) and Tomasella et al. (2003) were used, while, for the estimation of Ks and the $K(\theta)$ relationships, the equations tested were those of Tomasella and Hodnet (1997) (Table 2).

Tomasella et al. (2003) defined the term moisture equivalent (Me) as the gravimetric moisture content remaining in a disturbed soil sample after centrifuging at 2400 rpm for 30 min. Since moisture equivalent was not measured in this study, the average value reported by Tomasella et al. (2003) was considered.

Table 2. Pedotransfer functions for tropical soils that were evaluated

Pedotransfer functions for the $h(\theta)$ relations used in this study	
$\theta r = 0.308\ C$ $\ln(\alpha) = -0.627$ $\theta s = 84.1 - 0.206\ C - 0.322\ (S + Si)$ $m = 0.503 - 0.0027\ (Si + C) - 0.066\ OC + 0.0094\ CEC$	van den Berg et al. (1997)
$\theta r\ (\%) = 22.733 - 0.164\ S + 0.235\ CEC - 0.831\ pH + 0.0018\ C^2 + 0.0026\ S\ C$ $\theta s\ (\%) = 81.799 + 0.099\ C - 31.42\ \rho + 0.018\ CEC + 0.451\ pH - 0.005\ S\ C$ $\ln(\alpha)\ (x\ 100\ kPa^{-1}) = -2.294 - 3.526\ Si + 2.44\ OC - 0.076\ CEC - 11.331\ pH + 0.019\ Si^2$ $\ln(n)\ (x\ 100) = 62.986 - 0.883\ C - 0.529\ OC + 0.593\ pH + 0.007\ C^2 - 0.014\ S\ Si$	Hodnett and Tomasella (2002)
$X1 = -1.0679 + 0.0536107\ CS$ $\quad X2 = -1.17468 + 0.0808098\ S$ $X3 = -1.05976 + 0.0650437\ Si$ $\quad X4 = -2.10641 + 0.0427715\ C$ $X5 = -2.21391 + 8.92268\ Me$ $\quad X6 = -6.03516 + 4.81197\ \rho$ $Z1 = 4.25417\ X1 + 2.72322\ X2 + 3.07242\ X3 + 5.00093\ X4 - 0.195062\ X5 - 0.377081\ X6$ $Z2 = 0.110144 + 0.640373\ Z1 - 1.16884\ Z1^2 - 0.155394\ X4 - 0.358591\ Z1\ X4 - 1.00996\ Z1^2\ X4 + 0.126617\ X4^3$ $\alpha = 10^{(0.0736768 + 0.789068\ Z2)}$ $Z3 = 0.37398\ X1 - 0.0940338\ X1^3 + 0.838535\ X1\ X5 - 0.590525\ X1^2\ X5 + 0.76113\ X5^2 - 0.789465\ X1\ X5^2 - 0.273647\ X5^3 - 0.512764\ X6 - 0.455363\ X1\ X6 - 0.38428\ X1^2\ X6 + 0.731809\ X5\ X6 - 1.00484\ X1\ X5\ X6 - 0.172341\ X5^2\ X6 + 0.219746\ X6^2 - 0.367679\ X1\ X6^2 - 0.131251\ X6^3$ $Z4 = -0.360294 + 0.76878\ Z3 + 0.0770122\ Z3^3 - 0.193142\ X2 - 0.121583\ Z3\ X2 + 0.0889415\ Z3^3\ X2 + 0.284168\ X2^2 - 0.0674767\ X2^3 - 0.202897\ X3 - 0.341951\ Z3\ X3 - 0.270616\ X2\ X3 + 0.0880845\ X2^2\ X3 + 0.24982\ X3^2 + 0.102658\ X2\ X3^2 - 0.0801841\ X3^3$ $n = 10^{(0.140543 + 0.0797516\ Z4)}$ $Z5 = 0.164417 + 0.126139\ X1^2 + 0.281797\ X3 + 0.484823\ X1\ X3 - 0.293866\ X3^2 - 0.354924\ X1\ X3^2 - 0.705803\ X6 - 0.189153\ X3\ X6 - 0.267997\ X1\ X3\ X6 - 0.023954\ X3^2\ X6 - 0.0918816\ X1\ X6^2 + 0.0323997\ X6^3$ $\theta s = 0.515224 + 0.100899\ Z5$ $Z6 = 0.12867 - 0.492412\ X3 + 0.787425\ X5 - 0.235254\ X3\ X5$ $\theta r = 0.161487 + 0.101111\ Z6$	Tomasella et al. (2003)
Pedotransfer functions for the estimation of Ks and $K(\theta)$ relations used in this study.	
$Ks = 56540\ \varphi e^{4.5359}$ $\quad$ (mm h^{-1}) $\eta = 1.843\ b + 3.701$ $\quad$ (dimensionless) $K(\theta) = Ks\ Se^{\eta}$	Tomasella and Hodnet (1997)

ρ: bulk density (g cm^{-3}); OC: organic carbon (%); CEC: cation exchange capacity ($cmol_c\ dm^{-3}$; $cmol_c\ kg^{-1}$); CS: coarse sand fraction (>0.2 mm); S: sand fraction (50-200 µm); Si: silt fraction (2–50 µm); C: clay fraction (<2 µm); Me: moisture equivalent (%); φe: effective porosity (dimensionless), calculated as total porosity minus the water content at a matric potential of -33 kPa; b: parameter of the Brooks-Corey water retention curve. Se: effective saturation (dimensionless).

To assess the accuracy of the estimated parameter, the coefficient of determination r^2 and the square root of the mean squared error (SRMSEθ) values between the measured and simulated values were calculated at all depths of the soil profile. The values obtained were then compared to those found in the previous section.

RESULTS

h(θ) relationships

The van Genuchten equation parameters for the five soil depths under study are included in table 3. The r^2 and the SRMSEθ of the differences between the measured and estimated θ values at each depth of the soil profile are also included in table 3. The van Genuchten equation adapts well to the observed values for all depths, passing through the center of the set of points which show little dispersion with respect to the curve, in particular to the three lower depths of the soil profile (Figure 1). Luckner et al. (1989) defined θr as the soil water content at which water flow ceases in response to the hydraulic gradient, since the water molecules remain strongly adhered to the soil particles. Hodnett and Tomasella (2002) stated that θr is the water content for which the derivative of the function $\theta(h)$ is zero, but empathized that θr can, for most purposes, only be obtained by curve fitting. Thus, θr was initially optimized, obtaining a fitted value equal to zero in almost all cases, with the exception of at the 0.15 m depth, where a value of 0.2028 $cm^3\ cm^{-3}$ was obtained. However, the optimized 0.2028 $cm^3\ cm^{-3}$ value was greater than the smallest measured value of the soil moisture content at 0.15 m depth (0.1917 $cm^3\ cm^{-3}$). Consequently, and taking into account that the soil water content data measured in the field were far from the low values for which θr is defined, θr value was set equal to zero for all soil depths, and only α and m were optimized with the $h(\theta)$ data.

K(θ) relationships

In the determination of point values of K, cubic spline relationships for $H(z)$ and $\theta(z)$ were used. Cubic splines were adjusted by regression techniques to the H and θ data measured at different depths of the soil profile (z) for the days when the estimations of K were made. A cubic degree polynomial function was defined between each measurement depth. Cubic polynomial functions for $H(z)$ and $\theta(z)$ allowed the estimation of point values of K with the use of equations 12 and 13. The derivation of the $H(z)$ cubic spline also allowed to determine profile depths with zero water flux.

As an example, figure 2 illustrates the functional variation of the $H(z)$ and θ (z) relationships (Figures 2a and 2b, respectively) for the days May 4, 5 (in the morning) and May 6 (in the afternoon), 2018, including the point values of both relationships. Figure 2 shows how the values of the total head (Figure 2a) and the volumetric water content (Figure 2b)

Table 3. Parameters of van Genuchten's $h(\theta)$ equation and fitted l parameter of the $K(\theta)$ relationship

Soil depth	θs	α	m	n	r^2	SRMSEθ	l fitted value	SRMSEk
m	$cm^3\ cm^{-3}$	cm^{-1}				$cm^3\ cm^{-3}$		m day^{-1}
0.15	0.577	0.1024	0.1794	1.2186	0.65	0.02589	-8.59	0.000679
0.30	0.591	0.0835	0.1586	1.1886	0.62	0.02392	-9.92	0.000957
0.45	0.608	0.0295	0.1962	1.2442	0.87	0.01457	-7.04	0.000814
0.60	0.598	0.1019	0.1474	1.1729	0.77	0.01433	-11.2	0.001632
0.90	0.559	0.1638	0.1265	1.1449	0.72	0.01876	-13.26	0.000417

θs: saturated soil water content; α, m and n are parameters of the $h(\theta)$ van Genuchten equation; m and n are dimensionless. r^2: coefficient of determination between the measured and estimated θ values; SRMSEθ: square root of the mean squared error of the differences between the measured and estimated θ values; l: parameter of the $K(\theta)$ relationship (equation 13); SRMSEk: Square root of the mean squared error (SRMSE) between the measured and predicted K values.

decrease over time in the profile in the first two days due to soil drying processes, and later, on May 6, the water content is redistributed in the profile. Since a shallow water table is present in the study area, at a depth of approximately 1 m, permanent capillary rise was observed, whose influence in the form of the $H(z)$ and $\theta(z)$ relationships was evident, where the total head and the volumetric moisture content increase near the bottom of the soil profile. Near the soil surface, the moisture content and the total head tend to decrease due to evaporation. The behavior of H showed two zero-flux points as a consequence of the capillary rise of water: the first near the soil surface, which divides an

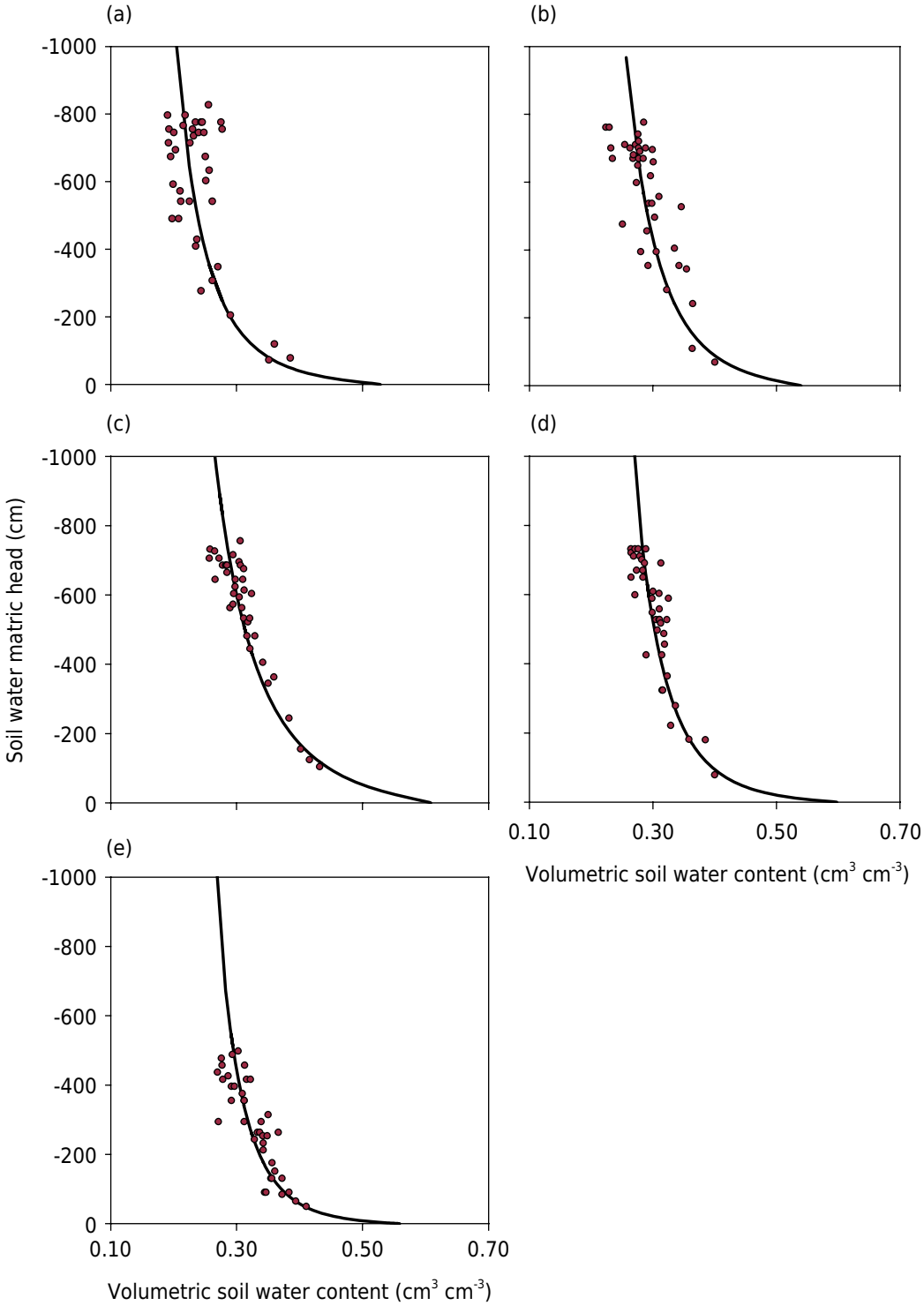

Figure 1. Representation of the $h(\theta)$ relationships of the soil profile: (a) 0.15 m depth; (b) 0.30 m depth; (c) 0.45 m depth; (d) 0.6 m depth; and (e) 0.9 m depth.

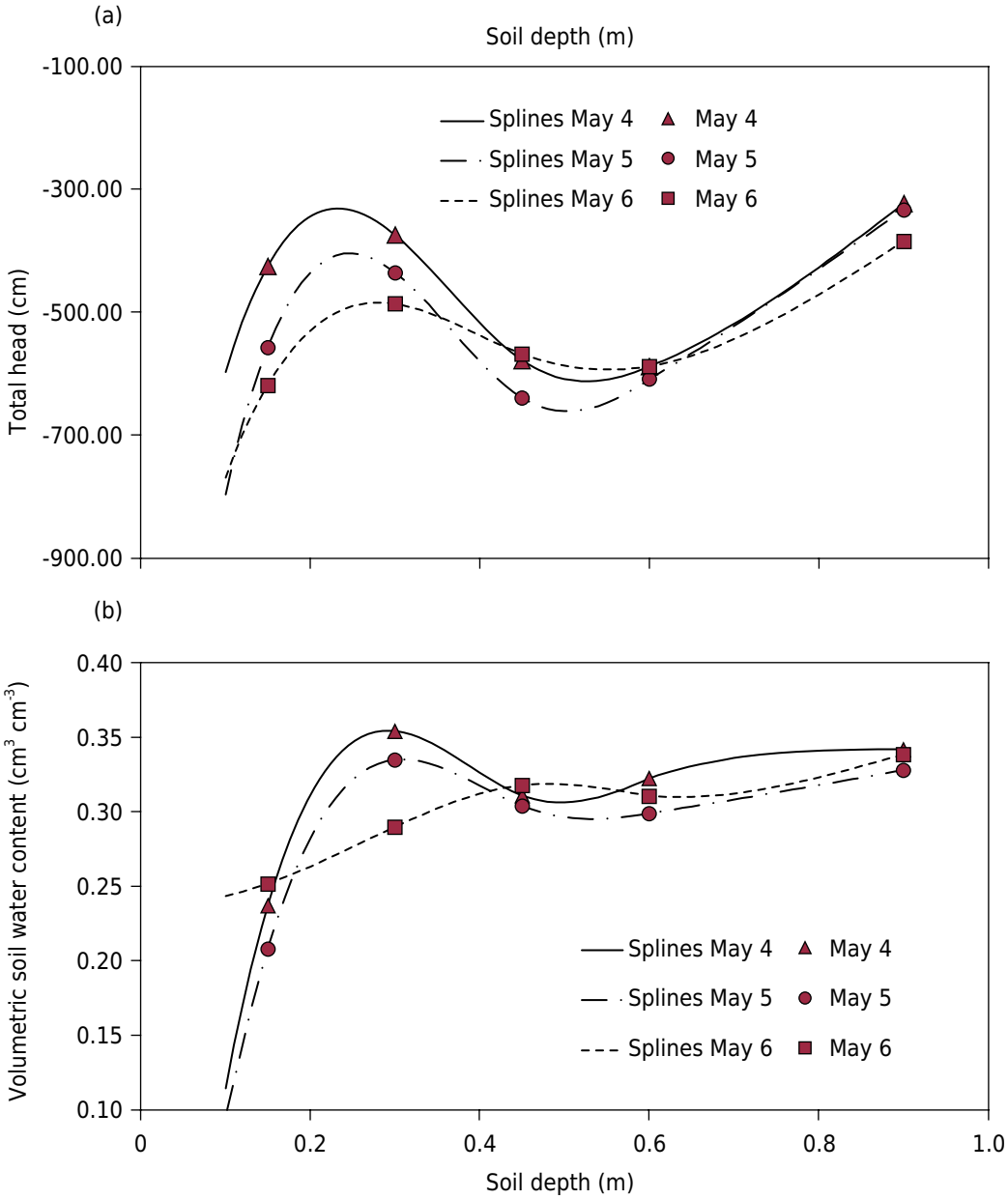

Figure 2. Measured values of total head *H* (a) and soil volumetric water content *θ* at different soil depths (b), and cubic splines functions for days 4, 5 and 6 May 2018.

evaporation zone from an infiltration zone; and a second, deeper in the profile, in which the infiltration zone converges with the capillary rise (Figure 2). Since there was no application of water by rain or irrigation to the soil surface, the downward vertical flow of the infiltration water induced downward movement of both zero-flux planes. If the process were to continue, the two zero-flux points would coincide at a single point at a later date, from which water movement would only be upward vertical from the phreatic table to the surface.

For the estimation of point values of *K*, equations 12 and 13 were applied for each measurement date. Cubic degree *θ*(*z*) polynomial functions were integrated from the depths *z1* under analysis (0.15, 0.30, 0.45, 0.60 and 0.90 m) to the depth or depths of the zero water flux on the analyzed day.

Equation 14, with the parameter *l* fixed at 0.5, underestimated the hydraulic conductivity in the soil profile for the five depths, although the numerical differences between the estimated and the predicted values of *K* never exceeded 0.0056 m day^{-1}. However, to have

a more precise estimate of the functional relationships $K(\theta)$ at the different depths, the value of parameter l in equation 14 was optimized over the point values determined for hydraulic conductivity in the five soil depths. As a result, negative values were obtained for l, which were included in figure 3, and shows the fit of equation 14 to the data. Table 3 shows the SRMSEk values between the measured and fitted K values at all soil profile depths, when the parameter l was optimized.

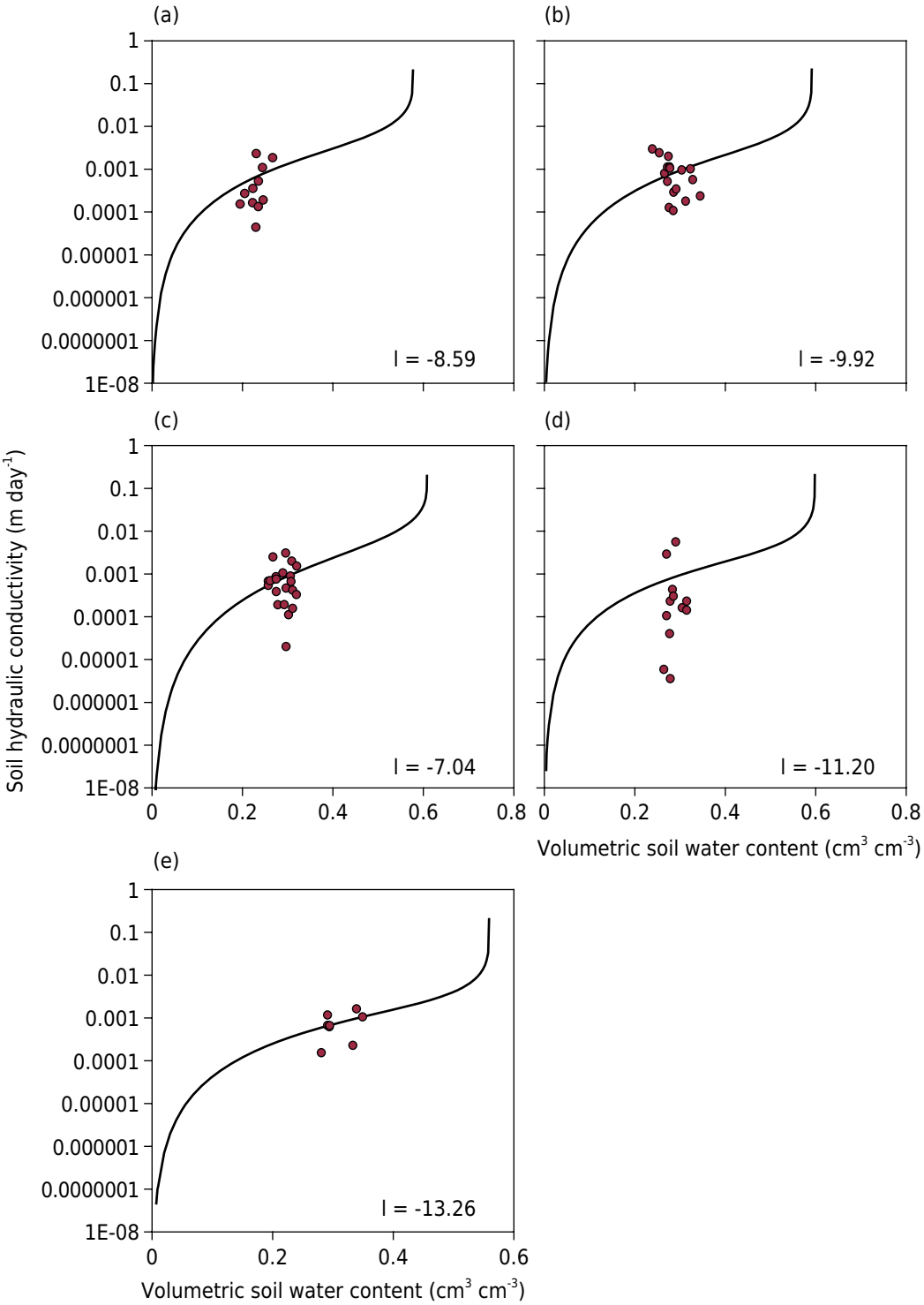

Figure 3. Comparison between the point values of soil unsaturated hydraulic conductivity (K), determined in this study, and the Mualem–van Genuchten $K(\theta)$ relationship (l fitted) for the different soil profile depths. (a) 0.15 m depth; (b) 0.3 m depth; (c) 0.45 m depth; (d) 0.6 m depth; and (e) 0.9 m depth.

Comparison of the *h*(θ) and *K*(*θ*) relationships obtained with estimates for the same relations derived from pedotransfer equations

Based on the physical properties of the soil profile, and with the use of pedotransfer equations presented in table 2, different sets of saturated hydraulic conductivity values and parameters of the *h*(*θ*) and *K*(*θ*) relationships were estimated. The results obtained were then graphically compared with the *h*, *θ* and *K* point values determined in this study, hereinafter referred to as "measured values", to verify their validity and applicability. As reported by Botula et al. (2012), little information has been generated about the validation of pedotransfer equations for tropical soils, highlighting this study's importance.

h(*θ*) relationships

The results obtained for the parameters of the van Genuchten *h*(*θ*) relationships (Equation 1) are summarized in table 4. To complete the comparison between the measured or fitted values of the parameters with those estimated with the soil pedotransfer equations, figure 4 shows the comparison between the measured point values of the *h*(*θ*) relationships with the functional curves constructed by using the pedotransfer estimated parameters.

K(*θ*) relationships

For the estimation of the *η* and *φe* parameters in the *K*(*θ*) equation proposed by Tomasella and Hodnet (1997) (Table 2), the Brooks and Corey equation for the *h*(*θ*) relationships was fitted to the data, as proposed by the same authors. The *Ks* values estimated by applying the equation proposed by these authors are included in table 5. Besides, figure 5 shows the comparison between the measured *K*(*θ*) values and the predicted *K*(*θ*) relationships by applying the pedotransfer equation proposed by Tomasella and Hodnet (1997) (equation in table 2, parameters in table 5).

Table 4. Parameters of the hydrodynamic characteristics *h*(*θ*) of the soil profile, estimated with the pedotransfer functions shown in table 2

Soil layer	θ_r	θ_s	α	*m*	*n*	SRMSE*θ*
m	——— $cm^3\ cm^{-3}$ ———		cm^{-1}			$cm^3\ cm^{-3}$
van den Berg et al. (1997)						
0.00-0.15	0.252	0.599	0.05237	0.536	2.155	0.02954
0.15-0.30	0.267	0.592	0.05237	0.560	2.275	0.03706
0.30-0.45	0.269	0.608	0.05237	0.564	2.291	0.05075
0.45-0.60	0.269	0.599	0.05237	0.579	2.376	0.03909
0.60-0.90	0.288	0.573	0.05237	0.604	2.528	0.04071
Hodnett and Tomasella (2002)						
0.00-0.15	0.377	0.598	0.03287	0.317	1.465	0.18555
0.15-0.30	0.382	0.589	0.03255	0.324	1.479	0.14808
0.30-0.45	0.396	0.606	0.03958	0.336	1.506	0.13353
0.45-0.60	0.390	0.595	0.03947	0.332	1.496	0.13538
0.60-0.90	0.384	0.561	0.03671	0.327	1.485	0.12018
Tomasella et al. (2003)						
0.00-0.15	0.196	0.640	0.14511	0.356	1.553	0.02853
0.15-0.30	0.196	0.624	0.16429	0.319	1.468	0.04841
0.30-0.45	0.216	0.662	0.14887	0.404	1.679	0.07766
0.45-0.60	0.216	0.650	0.14973	0.368	1.582	0.05500
0.60-0.90	0.209	0.600	0.16569	0.262	1.354	0.02262

*θ*r: residual soil water content; *θ*s: saturated soil water content; *α*, *m* and *n* are parameters of the *h*(*θ*) van Genuchten equation; *m* and *n* are dimensionless; SRMSE*θ*: square root of the mean squared error between the measured and estimated *θ* values.

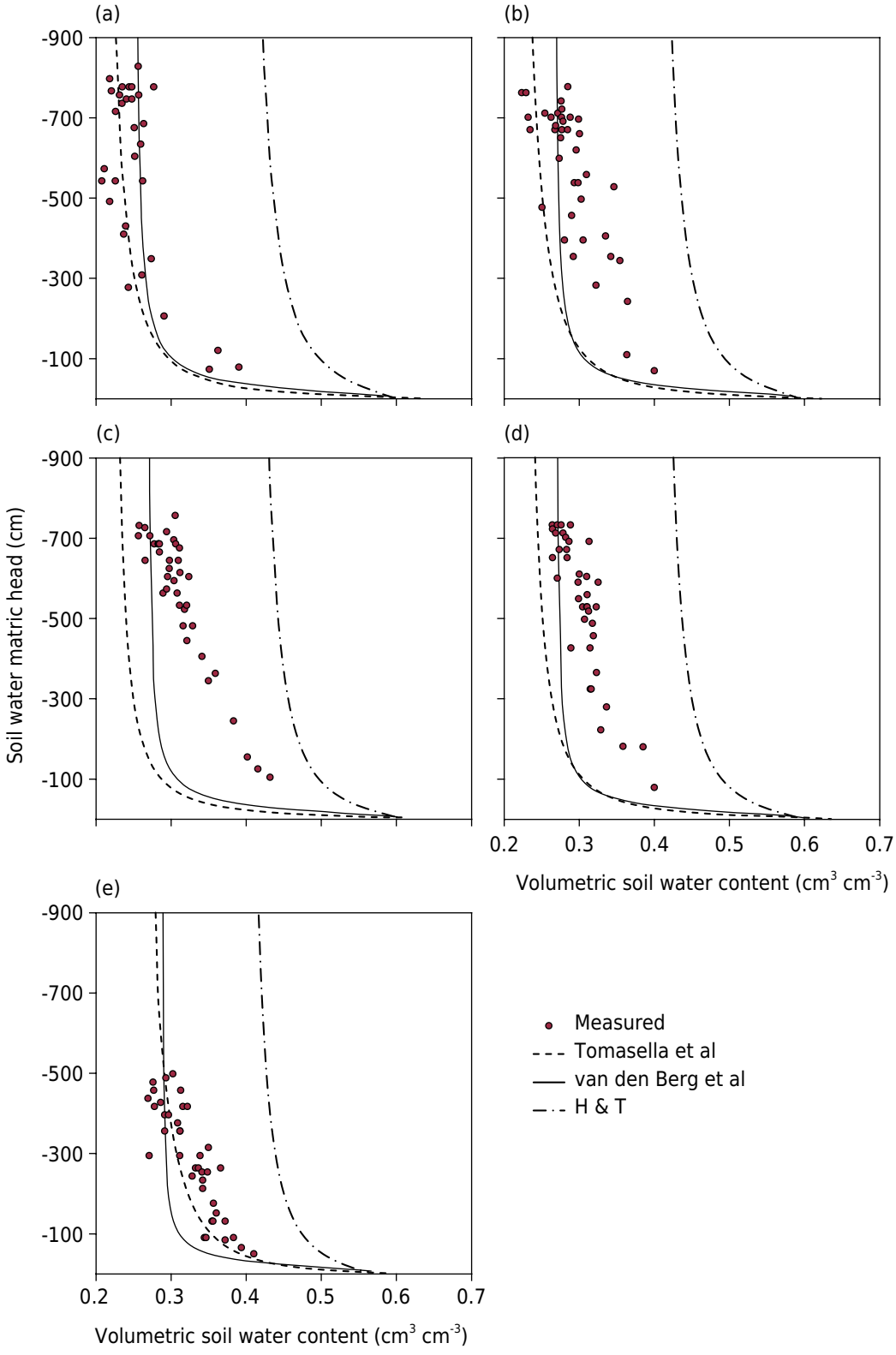

Figure 4. Functional relationships $h(\theta)$ of the soil profile obtained with pedotransfer equations and comparison with the point values determined in the present study. Tomasella et al refers to the equations proposed by Tomasella et al. (2003); van den Berg et al refers to the equations proposed by van den Berg et al. (1997); and H&T refers to the equations proposed by Hodnett and Tomasella (2002). (a) 0.15 m depth; (b) 0.30 m depth; (c) 0.45 m depth; (d) 0.60 m depth; and (e) 0.90 m depth.

Table 5. Measured and estimated *Ks* values, and parameter η in the $K(\theta)$ equation calculated as proposed by Tomasella and Hodnet (1997) for tropical soils

Soil layer	Measured *Ks*	Estimated *Ks*	Parameter η estimated	SRMSE*k*
m	——— m day^{-1} ———			m day^{-1}
0.00-0.15	0.2160	8.6537	12.284	0.000818
0.15-0.30	0.2280	5.2738	13.944	0.001324
0.30-0.45	0.2088	4.3915	11.953	0.000980
0.45-0.60	0.2184	5.0132	14.671	0.001789
0.60-0.90	0.2160	3.1410	16.815	0.000641

SRMSE*k* = Square root of the mean squared error between the measured and estimated *K* values.

DISCUSSION

h(θ) relationships

The r^2 and the SRMSEθ of the differences between the measured and estimated θ values were, in all soil layers, higher than 0.62 and lower than 0.02589 cm^3 cm^{-3}, respectively (Table 3). The saturated soil water content (θs), considered here numerically equal to the soil porosity, was slightly different among the soil depths (Table 3), what was proportional to the clay contents (Table 1). The lowest values of θs, determined for the depths of 0.15 and 0.90 m, were due to these soil depths having the lowest clay fraction (78 and 80 %, respectively). The θs value depends on the type and quantity of minerals present in the soil, and organic matter improves soil structure and thus modifies the soil's bulk density (Tuller and Or, 2005; Revil and Lu, 2013; Lu and Lu Khorshidi, 2015). The θs values estimated in this study were slightly greater than those reported by Lu (2016) for clay soils (θs = 0.57 cm^3 cm^{-3}), obtained under laboratory conditions, except for the depth of 0.90 m. The lowest value of α was observed at a depth of 0.45 m and the largest at a depth of 0.90 m (Table 3), the latter being attributed to the greater percentage of sand at that depth.

K(θ) relationships

The cubic splines that were used in the instantaneous profile method, and that were fitted to the $H(z)$ and $\theta(z)$ data measured at different depths of the profile, allowed for an estimation of the terms of equations 12 and 13, and allowed point estimates of K to be obtained, which were related to the soil water content to obtain pairs of values for the $K(\theta)$ relationship at each soil depth. Thus, the hypothesis of the study has been verified, stated as follows: "the instantaneous profile method, in which splines were used to express the variation of the total head and of the volumetric soil water content with depth, can be applied in tropical Vertisols, to determine the $K(\theta)$ relationships at different soil profile depths".

Moreover, concerning the relations $K(\theta)$, the results obtained of the adjustment of the Mualem-van Genuchten equation (Equation 14) over the points determined with the instantaneous profile method when the parameter l has been optimized, are completely acceptable (Figure 3), and this for all depths of the soil profile. Fitted negative values for the parameter l have also been reported by others: Schaap and Leij (2000) reported fitted l values were often negative, with an optimal value of -1. Schaap and van Genuchten (2006) fitted the parameter l and reported values from -0.4 to -5.51. In this study, the l values varied from -7.04 (0.45-m deep) to -13.26 (0.90-m deep).

Comparison of the *h*(θ) and *K*(θ) relationships obtained with estimates for the same relations derived from pedotransfer equations

h(θ) relationships

All of the pedotransfer equations tested tended to overestimate θs. The pedotransfer equations that allowed a closer approximation to the observed field values were those

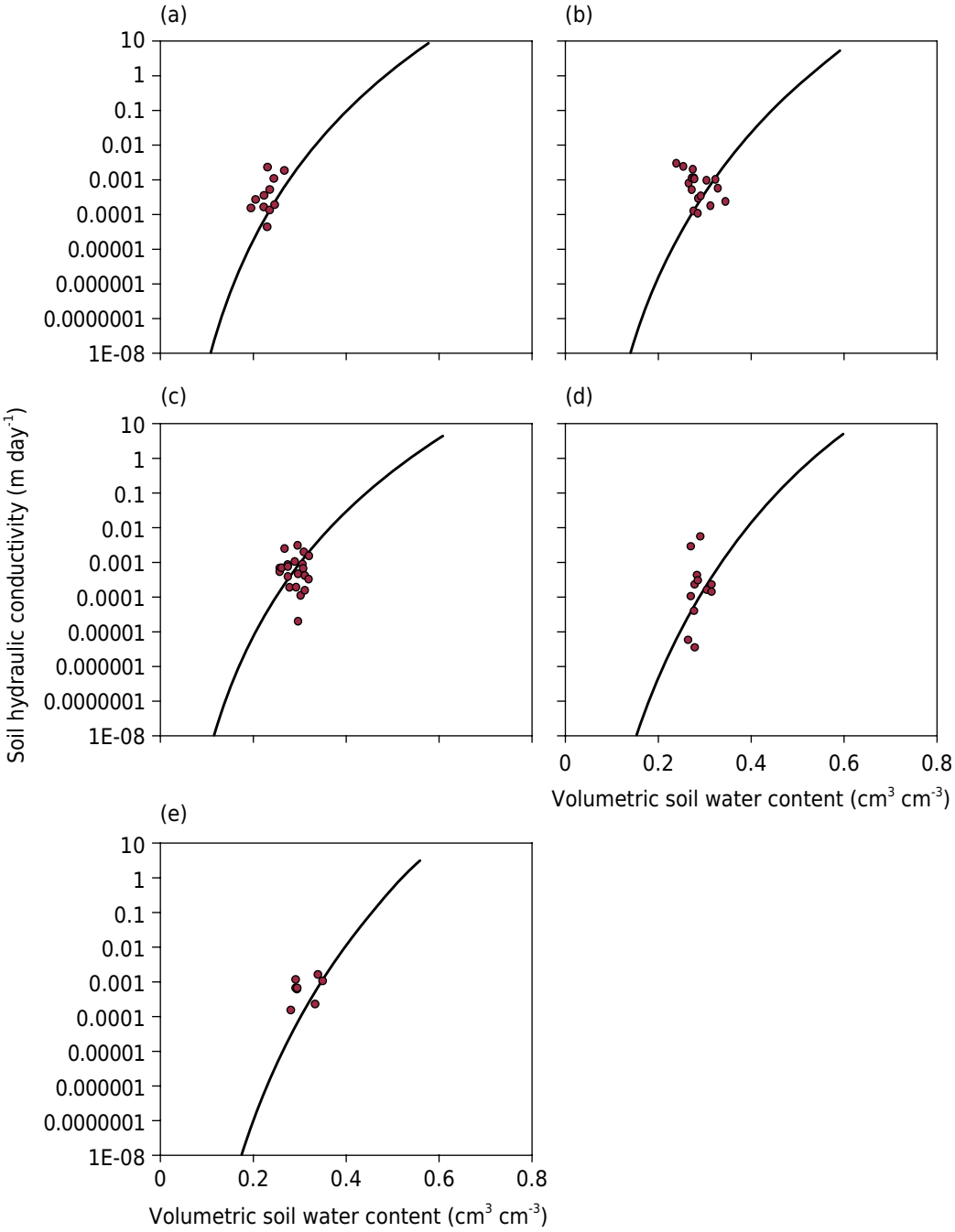

Figure 5. Comparison between the point values of soil unsaturated hydraulic conductivity (K) determined in this study, and the pedotransfer equation for $K(\theta)$ proposed by Tomasella and Hodnet (1997) for the different soil profile depths. (a) 0.15 m depth; (b) 0.3 m depth; (c) 0.45 m depth; (d) 0.6 m depth; and (e) 0.9 m depth.

proposed by van den Berg et al. (1997) and Hodnett and Tomasella (2002), and the equations proposed by Tomasella et al. (2003) predicted larger values for θs compared to those observed. A similar result was observed for m: all the tested equations overestimated their values, although in this case the equations proposed by van den Berg et al. (1997) were those which overestimated the m values the most. Finally, with regard to the parameter α, the equations proposed by Tomasella et al. (2003) tended to overestimate observed values, while those proposed by van den Berg et al. (1997) and Hodnett and Tomasella (2002) tended to underestimate half the values and overestimate the remaining half.

Figure 4 graphically shows that the pedotransfer equations proposed for tropical soils by van den Berg et al. (1997) and by Tomasella et al. (2003) approximated actual values

measured in this study. Specifically at the 0.15 and 0.9-m soil depths the equations proposed by Tomasella et al. (2003) closely matched to the measured values, which was supporting evidence of the efforts made by different authors to estimate the $h(\theta)$ relationships of soils. The SRMSEθ calculated at the 0.15-m depth was 0.029 cm^3 cm^{-3} and was 0.023 cm^3 cm^{-3} at the 0.9-m depth (Table 4), which were similar to the values of 0.026 and 0.019 cm^3 cm^{-3} respectively, determined when fitting van Genuchten's equation to the measured data for the same soil depths (Table 3). In the intermediate soil profile depths, results were more modest, but were still encouraging. The SRMSEθ values for the pedotransfer equations proposed by van den Berg et al. (1997) and by Tomasella et al. (2003) never reached values greater than 0.078 cm^3 cm^{-3} (Table 4). In contrast, the equations proposed by Hodnett and Tomasella (2002) were those that deviated the most from the values determined in the field, where SRMSEθ values were greater than 0.12 cm^3 cm^{-3} in all cases. This result highlights the need for further research in order to propose new, more efficient pedotransfer equations for tropical soils (Botula et al., 2012).

K(*θ*) relationships

The *Ks* values estimated by applying the equation proposed by Tomasella and Hodnet (1997) greatly overestimated the measured values in all cases (Table 5). Results confirmed the need to calibrate pedotransfer equations to predict $K(\theta)$ relationships in tropical soils, for which there are practically no such studies. In contrast, although the *Ks* values were greatly overestimated at all depths of the soil profile, the predicted $K(\theta)$ values were close to those estimated with the instantaneous profile method. The results were encouraging and underline the potential for using pedotransfer equations to estimate the soil $K(\theta)$ relationship. In all cases, the SRMSE*k* values (Table 5) were less than 0.0018 m day^{-1}, which were close to the values determined during optimization of the *l* parameter. The biggest difference between the SRMSE*k* values calculated here compared to those calculated during the optimization of the *l* parameter, 0.000367 m day^{-1}, was observed at the 0.30 m depth (Tables 3 and 5).

CONCLUSIONS

The hypothesis of the study has been verified: the use of cubic splines to represent the spatial variation of the $H(z)$ and $\theta(z)$ relations in the application of the instantaneous profile method allowed point estimates of K to be obtained, which were related to the volumetric moisture content in the soil profile, to obtain pairs of values for the $K(\theta)$ relationship. In addition, $h(\theta)$ relationships were constructed for the five depths of the soil profile, so that hydrodynamic characterization of a tropical Vertisol at field conditions was performed.

Fitted, negative values of the *l* parameter in the Mualem–van Genuchten $K(\theta)$ equation were obtained, ranging from –7.04 (0.45-m depth), to -13.26 (0.90-m depth). With these *l* values, the Mualem–van Genuchten equation approximated the data for the $K(\theta)$ relationships very well in all soil profile layers.

Estimation of the $h(\theta)$ relationships with the use of pedotransfer functions proposed by Tomasella et al. (2003) were similar to the measured values at the 0.15 and 0.9-m soil depths, which supports efforts made by different authors to estimate the $h(\theta)$ relationships of soils on the basis of their physical and chemical properties. Although the *Ks* values estimated by applying the equation proposed by Tomasella and Hodnet (1997) have been greatly overestimated at all depths of the soil profile, the predicted $K(\theta)$ relationships pass over the points estimated with the instantaneous profile method. However, the results obtained by applying the rest of the pedotransfer equations that were tested in this study, for tropical soils, were not satisfactory, probably as a consequence of not taking into account the effects of macroporosity, typical of Vertisols. This underlines the need for further research to propose new, more efficient pedotransfer equations for tropical Vertisols, which consider the effects of macroporosity in the $K(\theta)$ relationships.

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