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Pedotransfer functions for estimating soil water retention curve of Sicilian soils” by Mirko Castellini and Massimo Iovino

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Abstract

Pedotransfer functions (PTFs) make use of routinely surveyed soil data to estimate soil properties but their application to soils different from those used for their development can yield inaccurate estimates. This investigation aimed at evaluating the water retention prediction accuracy of eight existing PTFs using a database of 217 Sicilian soils exploring 11 USDA textural classes. PTFs performance was assessed by root mean square differences (RMSD) and average differences (AD) between estimated and measured data. Extended Nonlinear Regression technique (ENR) was adopted to recalibrate or develop four new PTFs and Wind's evaporation method was applied to validate the effectiveness of the relationships proposed. PTFs evaluation resulted in RMSD and AD values in the range 0.0630-0.0972 cm³ cm⁻³ and 0.0021-0.0618 cm³ cm⁻³, respectively. Best and worst performances were obtained respectively by PTF-MI and PTF-ZW. ENR allowed to recalibrate PTF-MI and PTF-ZW with improvements of RMSD (0.0594 and 0.0508 cm³ cm⁻³) and

to develop two relationships that improved RMSD by 75-78% as compared to PTF-MI. The results confirmed the potential of ENR technique in calibrating existing PTFs or developing new ones. Validation conducted with an independent dataset suggested that recalibrated/developed PTFs represent a viable alternative for water retention estimation of Sicilian soils.

Key words: parametric pedotransfer functions, water retention models, evaporation method, extended nonlinear regression technique, pedotransfer functions recalibration

Introduction

Knowledge of soil water retention curve, namely the relationship between soil water pressure head, h , and volumetric water content, θ , is important for agro-environmental modelling (Ventrella et al. 2012; Castellini et al. 2016; da Silva et al. 2017a) or for irrigation scheduling and optimization (Katerji et al. 2013; Rallo et al. 2018).

Several methods are available in the literature to estimate the $\theta(h)$ such as sand-box or hanging water column apparatus (Burke et al. 1986), pressure plate apparatus (Dane and Hopmans 2002) or evaporation method (Wind 1968). However, because of soil spatial variability, direct measurements of soil water retention are expensive, time consuming and require complex measurement devices and skilled operators which make them practically unfeasible at the scale of irrigation district (Sinowski et al. 1997). As a result, there is a great interest in developing alternative estimation methods or experimental procedures that are easy to apply, inexpensive, conceptually robust and relatively accurate (da Silva et al. 2017b; Castellini et al. 2018).

Pedotransfer functions (PTFs) predict the soil water retention from easily measured and/or routinely surveyed soil data such as particle size distribution, organic carbon content and bulk density. Being user-friendly and parsimonious in terms of input variables, PTFs have been implemented in various models as well as in public domain software frameworks to simulate the behaviour of complex agricultural systems (Donatelli 2014; Jones et al. 2016). More recently, for example, da Silva et al.

(2017a) applied PTFs to identify the spatial variability of key variables related to soil water retention (i.e., available water capacity, field capacity, and permanent wilting point), as well as important hydrodynamic soil properties (unsaturated hydraulic conductivity and diffusivity), in a Brazilian sandy soil under a fallow management.

The $\theta(h)$ curve may be estimated using existing or specifically developed PTFs (Vereecken et al. 2016; Van Looy et al. 2017). The first experimental approach is more widely used. The first step in this strategy is the selection of appropriate PTFs for estimating the water retention curve (Van Looy et al. 2017). However, as most of available PTFs were developed empirically, their applicability may be limited to the data used to define them and their use for other soils may yield unreliable predictions (Wösten et al. 2001). Therefore, a preliminary evaluation and, eventually, a recalibration is necessary (Rustanto et al. 2017).

The accuracy of PTFs can only be evaluated using independent data sets (Schaap 2004). This means that users should preliminarily gather a data set and test several PTFs in order to decide whether or not a particular PTF is suitable for a particular application. However, the lack of truly representative information on soil hydraulic characteristics is the main drawback to PTFs validation in certain areas. In particular, soil databases contain mainly results for soils of Northern Europe and Northern America, whereas validation for soils of the Mediterranean region is very limited (Goncalves et al. 1997). This can be the reason why evaluations of the PTFs applicability in relatively unexplored geographical areas have been continuously conducted even in the very last years (Buccigrossi et al. 2010; Abbasi et al. 2011; Barros et al. 2013; Medeiros et al. 2014; Kupec et al. 2015; Xiangsheng et al. 2016; Rustanto et al. 2017). In other words, although several PTFs were proposed in the literature, relatively little information is available about their performance, and comparisons between measured and estimated water retention data is of crucial importance to determine their applicability (i.e., reliability and precision, as a function of considered pressure head interval) for a wide range of soil textures.

With the aim to evaluate the accuracy in predicting the soil water retention characteristics for Sicily, some widely used PTFs (Saxton et al. 1986; Rawls and Brakensiek 1989; Vereecken et al. 1989; Scheinost et al. 1997; Minasny et al. 1999; Wosten et al. 1999; Saxton and Rawls 2006; Zacharias and Wessolek 2007) were tested using a data set of about two hundred soils, specifically collected, and characterized by different texture, pedology and land use. In order to provide more accurate estimates of the van Genuchten model parameters (van Genuchten 1980), two existing parametric PTFs were recalibrated by the Extended Nonlinear Regression technique. Two new PTFs were also developed using only soil texture and organic carbon content as input variables. Reliability of recalibrated and specifically developed PTFs was tested with independent water retention data measured, for seven differently textured Sicilian soils, by the Wind's evaporation method.

Materials and methods

Description of pedotransfer functions

A PTF is a function that has as arguments basic data describing the soil (e.g., particle size distribution, bulk density and organic carbon content) and yields as a result unknown soil property, as the soil water retention function (Tietje and Tapkenhinrichs 1993). In detail, the soil water retention function may be determined by estimating discrete water content values, θ_i , at specific pressure heads, h_i , or by estimating the parameters of selected closed-form analytical functions $\theta(h)$ (Romano and Santini 1997). The former method is referred to as the Point Regression Method and the latter one as the Functional Parameter Regression Method (Tietje and Tapkenhinrichs 1993). The Point Regression Method may result in non-monotonic retention functions mainly when water contents are calculated from different regressor variables at different pressure head values or when prediction is carried out for soils differing from those included in the calibration database. The PTFs that estimate the retention function parameters are easier to use for modeling purposes than the point PTFs (Tietje and Tapkenhinrichs 1993).

Eight PTFs were selected from literature and evaluated in this study (**Table 1**). Selection of PTFs was conducted according to their reliability, as established in previous investigations (Patil and Singh 2016), as well as to previous validations conducted under different conditions (Tietje and Tapkenhinrichs 1993; Romano and Santini 1997). In particular, the PTFs proposed by Saxton et al. (1986), Saxton and Rawls (2006), Rawls and Brakensiek (1989), Vereeken et al. (1989), Wösten et al. (1999), Scheinost et al. (1997), Minasny et al. (1999) and Zacharias and Wessolek (2007) were considered. All selected PTFs were characterized by input data that are easily gathered by common soil survey (i.e. soil texture, organic matter content and bulk density). Moreover, they were deduced from extensive databases of soils (Minansy et al. 1999; Rawls et al. 1982; Wösten et al. 1999).

The PTFs by Saxton et al. (1986) (PTF-S1) and Saxton and Rawls (2006) (PTF-S2) (**Table 1**) describe the water retention function with three equations for different pressure head subranges, and strictly speaking cannot be considered as a Functional Parameter Regression Method. In particular, the following relationships were considered: i) a constant water content equal to the saturated water content, θ_s , for pressure head ranging from zero to the air entry pressure head, h_b , that is itself estimated from soil physical attributes; ii) a linear relationship from h_b to an intermediate pressure head fixed to -102.0 cm (PTF-S1) or -336.6 cm (PTF-S2); iii) an exponential function for h values lower than -102.0 cm (or -336.6 cm). The database of soil attributes used to develop the PTF-S1 included a very extensive set of 2541 soil horizons (Rawls et al. 1982). The derived expressions are applicable to soils with the following ranges of clay, Cl , and sand, Sa , contents (USDA classification): $5\% \leq Sa \leq 30\%$ if $8\% \leq Cl \leq 58\%$ and $30\% \leq Sa \leq 95\%$ if $5\% \leq Cl \leq 60\%$. As compared to PTF-S1, a wider dataset of approximately 4000 soil water characteristics was used to derive the PTF-S2 which is applicable for $Cl < 60\%$ and organic matter content, OM , lower than 8%. The PTF from Rawls and Brakensiek (1989) (PTF-RB) estimates the parameters of the Brooks and Corey (1964) retention function (**Table 1**). The regression equations were based on the same database from Rawls et al. (1982) and are valid for $5 \leq Sa \leq 70\%$ and $5 \leq Cl \leq 60\%$. The European soil database HYPRES was used by Wosten et al. (1999) to develop a PTF (PTF-HY) to estimate

the parameters of the van Genuchten's water retention function (van Genuchten et al. 1980) (**Table 1**). A modified form of the van Genuchten function was used by Vereecken et al. (1989) (PTF-VE) to develop PTFs for Belgian soils with $Cl < 54.5\%$, $Si < 80.7\%$, $5.6 < Sa < 97.8\%$, organic carbon content, $OC < 6.6\%$ and bulk density, $1.04 < \rho_b < 1.23 \text{ g cm}^{-3}$. Scheinost et al. (1997) applied the Extended Nonlinear Regression (ENR) to a dataset of 87 soils to estimate the parameters of the van Genuchten function (PTF-SC) (**Table 1**). In particular, under the hypothesis that the pore-size distributions and the particle-size distributions are congruent (Arya and Paris 1981), parameters α and n may be estimated from, respectively, the geometric mean particle-size diameter, d_g , and the geometric standard deviation, σ_g (Shirazi and Boersma 1984). ENR approach was also applied by Minasny et al. (1999) with reference to 842 soil samples obtained in 218 Australian soil profiles (PTF-MI) and by Zacharias and Wessolek (2007) (PTF-ZW). In the former case, knowledge of d_g and σ_g , soil porosity ϕ , and percentages of soil particles with $d \leq 2 \text{ }\mu\text{m}$ and $2 < d \leq 20 \text{ }\mu\text{m}$ is required. In the second case, independent variables are Cl , Sa and OC (**Table 1**).

In summary, the eight PTFs chosen in this investigation are characterized by an increasing level of required input information: texture fractions for PTF-S1, texture fractions plus bulk density or soil porosity for PTF-RB, PTF-MI and PTF-ZW, texture fractions plus bulk density and organic carbon content for PTF-S2, PTF-VE, PTF-HY and PTF-SC.

Soil database and application of pedotransfer functions

Application of PTFs was carried out using a data set of 217 Sicilian soils characterized by a wide variation of the main soil physical properties (**Table 2**). Soil samples were extensively collected in three areas and in other 18 spot sites distributed in Sicily (Weynants et al. 2013). The first sampling is the wine-specialized area of Menfi (western Sicily). Upper horizon of 84 sites were sampled in an area of approximately 850 ha. The second sampling area is the irrigation district of Dirillo (southern Sicily). The data set consists of 61 soil samples collected in the A and B horizons of 29 soil profiles distributed in a 3000 ha area characterized by different pedology and land use. The third sampling

area is close to Santa Ninfa (western Sicily) in a 140 ha environmental protection area. A total of 54 sampling points were established in six plots including both agricultural (vineyard, olive grove, durum wheat cultivation) and natural vegetation (woodlot of eucalyptus trees, pine forest and Mediterranean maquis). Finally, distributed soil sampling was conducted in the A horizon of different sites characterized by both agricultural ($n = 13$) and forest ($n = 5$) land uses.

For each soil, the particle size distribution (PSD) was determined by the hydrometer method for particles having diameters, $d < 74 \mu\text{m}$ and by sieving for particles with $74 \leq d \leq 2000 \mu\text{m}$ (Gee and Or 2002). A total of 14 particle size fractions were determined that allowed to estimate d_g and σ_g according Shirazi and Boersma (1984). The clay, Cl , silt, Si , and sand, Sa , percentages were determined according to the USDA classification. The organic carbon, OC , content was determined by the Walkley-Black method (Nelson and Sommers 1996). Where required, the organic matter, OM , content was estimated to be 1.724 times OC . The selected 217 soils fall within 11 of the 12 textural classes of USDA (**Figure 1**) and the most represented classes are those of sandy-loam (55 soils), loam (44) and silty-loam (38). Bulk density or organic carbon values account for a wide range of variation (**Table 2**).

Soil water retention data for h values ranging from -0.05 to -1.50 m were determined on undisturbed soil cores (0.08 m in diameter by 0.05 m in height) by a hanging water column apparatus (Burke et al. 1986). At the end of experiment, the undisturbed soil cores were used to determine the dry bulk density, ρ_b (g cm^{-3}). Soil porosity, ϕ ($\text{cm}^3 \text{cm}^{-3}$), was calculated from ρ_b assuming a particle density of 2.65 g cm^{-3} . For each sampling point, sieved soil was packed to the ρ_b value of the undisturbed core in rings having a diameter of 0.05 m and a height of 0.01 m. These soil samples were used to determine the soil water content corresponding to $h = -3.37, -10.2, -30.6$, and -153.0 m by a pressure plate apparatus (Dane and Hopmans 2002). Statistics for $\theta(h)$ data are listed in **Table 2**. For each considered soil, optimized values of parameters α , n , θ_s and θ_r of the van Genuchten retention model were estimated by the RETC software (van Genuchten et al. 1991).

Development and testing of pedotransfer functions

Development of specific pedotransfer functions for Sicilian soils was carried out by the Extended Nonlinear Regression technique (ENR) (Scheinost et al. 1997; Minasny et al. 1999; Zacharias and Wessolek 2007; Weynants et al. 2009). Minasny et al. (1999) showed that ENR technique is more appropriate if compared with multiple regression method since the latter can give rise to PTF over-parameterization, due to the recognized correlation among parameters of van Genuchten model (Scheinost et al. 1997). A two-step preliminary statistical analysis is necessary to properly apply the ENR approach: i) using existing models or specifically derived regressions models, appropriate relationships are established between parameters α , n , θ_s and θ_r and physico-chemical soil properties (Cl , Si , Sa , d_g , σ_g , ρ_b , ϕ , OC), in which a number of unknown coefficients appears; ii) the aforementioned regression equations are then implemented into the selected $\theta(h)$ function and the corresponding unknown coefficients estimated through a non-linear optimization technique which minimizes the sum of squared residues between estimated and measured soil water retention data. To establish regressions models for Sicilian data set a multiple correlation analysis was performed between the selected physico-chemical soil properties (Cl , Si , Sa , d_g , σ_g , ρ_b , ϕ , OC) and the optimised parameters of the van Genuchten model. The ENR procedure was implemented into a Microsoft Excel worksheet.

Seven Sicilian soils differing in soil texture from sand to clay (**Figure 1**), were sampled to assess the performances of the recalibrated/developed PTFs. In particular, at each sampling site, two soil cores (0.075 m in height by 0.075 m in diameter) were collected in the soil surface layer (0-0.10 m) to determine the soil water retention in the laboratory by the evaporation method (Wind et al. 1968). After being equilibrated to a pressure head value of -0.10 or -0.20 m, depending on the soil texture (Bagarello et al. 2007), the soil core was sealed at the bottom to prevent water loss and submitted to a forced evaporation. Soil water pressure head was measured by ceramic micro-tensiometers horizontally placed at the center of three equally spaced soil core compartments. Soil water content

was measured by a scale with 0.01 g accuracy. Simultaneous measurements of h and θ were conducted every hour until the air entry pressure head of the uppermost tensiometer was exceeded. An iterative procedure, implemented in the code Metronia v. 3.04 (Halbertsma and Veerman 1994), allowed to obtain from 25 to 356 θ - h independently measured data pairs, within a pressure head range of about -0.1 to -5.5 m, that were compared with the corresponding values estimated by PTFs.

Evaporation method has been subject in the past to several experimental validations and improvements (Wendroth et al. 1993; Romano and Santini 1997; Bezerra-Coelho et al. 2018) so that it may be considered a reference method for evaluating indirect techniques for soil water retention estimation (Siltecho et al. 2015; Castellini et al. 2018). Moreover, compared to the equilibrium tensiometric and pressiometric methods that yield a limited number of θ - h pairs at pre-established pressure head values, the evaporation method allows validation of the selected PTFs with a large number of θ values in a range of pressure heads ($-0.1 \leq h \leq -7.0$ m) that is of specific interest for simulating water flux in unsaturated soils. Therefore, at least two advantages can be hypothesized in application of evaporation method: i) it allows to obtain a relatively high number of θ - h pairs with a single experiment; ii) it provides measurements of soil water retention from a depletion experiment involving an upward water flux that is more representative of natural hydrological processes. As a consequence, validation of PTFs conducted with retention data measured by the evaporation method can be considered relatively more reliable than those obtained by classical equilibrium approaches.

Evaluation of PTFs performance

Analysis of the PTFs performances was carried out applying the approach used by Minasny et al. (1999), that is based on the calculation of the root mean square deviation, RMSD:

$$RMSD = \sqrt{\frac{\sum_{i=1}^n (\theta_{pi} - \theta_{mi})^2}{n}} \quad (1)$$

being θ_{pi} and θ_{mi} , respectively, the estimated and measured values of the water content and n the total number of measured θ values. However, in order to detect any systematic bias in the θ estimation, the mean deviation, AD, was also calculated (Wösten et al. 2001):

$$AD = \frac{\sum_{i=1}^n (\theta_{pi} - \theta_{mi})}{n} \quad (2)$$

Validation of proposed PTFs for Sicilian soils (i.e., recalibrated/developed PTFs) was also conducted by linear regression analysis. The statistical significance of the correlation coefficient, R , between θ_{pi} and θ_{mi} was assessed by a *one-tailed t-test* ($p = 0.05$) and the 95% confidence intervals for the intercept and the slope of the liner regression line were calculated. The statistical significance of the differences between measured and estimated soil water content values was assessed by a *two-tailed paired t-test* ($p = 0.05$).

Results and discussion

Among the PTFs considered in this investigation, the most satisfactory result for Sicilian soils ($RMSD = 0.0630 \text{ cm}^3 \text{ cm}^{-3}$) was provided by PTF-MI that needs information on soil texture and bulk density (**Table 3**). Slightly less satisfactory results were provided by PTF-HY and PTF-VE ($RMSD = 0.0680 \text{ cm}^3 \text{ cm}^{-3}$) which in addition require the knowledge of OC . This confirms the literature findings that a relatively higher number of input variables does not necessarily return a more satisfactory estimation of soil water retention (Cornelis et al. 2001). Generally less reliable estimates were obtained when only the soil texture was used, i.e. PTF-S1 ($RMSD = 0.0752 \text{ cm}^3 \text{ cm}^{-3}$). On the other hand, low performances were obtained with PTF-ZW and PTF-SC that requires a relatively complete information (**Table 3**); this is probably a consequence of the limited data set used for their development. In other words, the best match between estimated, θ_p , and measured, θ_m ,

soil water retention data in terms of RMSD, can be obtained with PTFs which involve the knowledge of additional soil data besides soil texture. In some cases, the comparison between θ_p and θ_m showed a systematic bias in θ estimates (**Figure 2**). This bias was clearly detectable especially for PTF-ZW and PTF-SC, for which the highest AD values were found (**Table 3**), but was also relatively high for PTF-HY and PTF-VE, which conversely provided relatively low RMSD values compared to the other PTFs.

Results of PTFs evaluation were in agreement with literature findings. For a broad range of soils in Germany, Tietje and Tapkenhinrichs (1993) found an overall good performance of PTF-VE with a mean RMSD value of $0.0531 \text{ cm}^3 \text{ cm}^{-3}$, very close to the value obtained in this evaluation. In their case, PTF-VE also resulted in a general underestimation of the water content ($\text{AD} = -0.0145 \text{ cm}^3 \text{ cm}^{-3}$). An evaluation of the performances of PTF-RB and PTF-VE conducted by Romano and Santini (1997) showed that the soil water retention curve was slightly better estimated using the PTF proposed by Vereecken et al. (1989) close to saturation, whereas the two PTFs were comparable for $h = -10$ and -100 kPa. Moreover, these authors highlighted that the largest deviations between θ_p and θ_m were chiefly associated to those samples having low sand content and/or low values of bulk density. Ungaro and Calzolari (2001) reported a higher performance of PTF-S1 as compared to PTF-RB and PTF-VE (mean RMSD equal to 0.0698, 0.0882 and $0.0915 \text{ cm}^3 \text{ cm}^{-3}$, respectively). However, this behavior could be attributed to the particular characteristics of the validation data set. Also with our soils, PTF-S1, that uses two textural fractions, performed better than PTF-RB, using two textural fractions plus porosity (**Table 3**). For PTF-VE, Medeiros et al. (2014) reported RMSD values in the range $0.07\text{-}0.10 \text{ cm}^3 \text{ cm}^{-3}$, depending on the considered pressure head value. Application of PTF-VE, PTF-HY and PTF-SC to Belgian soils conducted by Cornelis et al. (2001) resulted in relatively better performances than for the case of Sicilian soils (RMSD equal to 0.0412, 0.0518 and $0.0573 \text{ cm}^3 \text{ cm}^{-3}$, respectively). The accuracy of these PTFs was further improved when they were applied exclusively to soils that fell within the database

calibration intervals (Cornelis et al. 2001). In summary, application of the selected PTFs to Sicilian soils provided estimates of soil water retention in agreement with literature findings despite some PTFs (PTF-VE, PTF-HY and PTF-MI) performed better than the remaining ones (**Table 3**).

According to literature (Manrique and Jones 1991; Heuscher et al. 2005; Zacharias and Wessolek 2007), a statistically significant correlation ($R^2 = 0.26$; $p < 0.05$) was found between ρ_b and OC for the Sicilian soils suggesting that inclusion of both variables was not necessary in the development of PTFs by the ENR techniques. Organic carbon determination can be easily conducted by standard laboratory equipment and it does not require collection of undisturbed soil samples. Determination of ρ_b is conversely more prone to compaction that accidentally occurs during sampling and to soil spatial variability as in the case, for example, of machinery traffic. For these reasons, only OC was retained for the aim of developing specific PTFs for Sicilian soils.

Application of ENR technique was carried out using selected relationships between the parameters of the van Genuchten model and the physico-chemical properties of the soil. In particular, statistically significant correlations between each parameter of the van Genuchten model and the selected independent variables were established by both linear and non-linear relationships derived from the literature (Vereecken et al. 1989; Scheinost et al. 1997; Minasny et al. 1999; Zacharias and Wessolek 2007) and/or specifically developed on the basis of the preliminary statistical analysis. In any case, simple relationships were considered, i.e., characterized by a limited number of unknown coefficients, in order to limit the risk of PTF over-parameterization. **Table 4** reports the relationships between the parameters of the van Genuchten model and the soil properties specifically developed from the database of Sicilian soils (PTF1 to PTF4). In particular, the approaches referred to as PTF1 and PTF2 make use of the same relationships proposed, respectively, by Minasny et al. (1999) (PTF-MI) and Zacharias and Wessolek (2007) (PTF-ZW). For these two cases, a recalibration of the original relationships was basically carried out by applying the ENR technique. Despite the relatively lower performance of PTF-ZW for Sicilian soils (**Table 3**), this PTF was selected to show the potential of recalibration in improving the PTF

prediction for a given region. PTF3 and PTF4 rely on linear and non-linear relationships between parameters α , n , θ_s and θ_r and independent variables Cl , Sa and OC that were specifically detected for the Sicilian soil database.

The results showed that a recalibration of the original relationships by Minasny et al. (1999) (PTF-MI) and Zacharias and Wessolek (2007) (PTF-ZW), respectively PTF1 and PTF2, determined a significant improvement in statistics (**Table 3**). In particular, although a slight improvement was obtained in recalibrating the PTF-MI, that is to say of a factor of 1.06 in terms of RMSD and a factor of 4.12 for AD, recalibration of PTF-ZW showed a noticeable improvement in RMSD (by a factor 1.91) and in AD values (by two order of magnitude) (**Table 3**). This confirms recent findings of literature which suggest a proper calibration of existing PTFs as a preferable solution to their direct application (Rustanto et al. 2017). However, since a clear improvement in soil water retention estimation was obtained only for one of the two recalibrated PTFs, our results also confirm that assessing the real accuracy of given PTFs for a specific environment needs comparisons with adequate sets of measured data. More satisfactory results were generally obtained with specifically developed PTFs yielding RMSD values of 0.0491 and 0.0470 $\text{cm}^3 \text{cm}^{-3}$, respectively for PTF3 and PTF4 ($AD = 0.0092\text{-}0.0002 \text{ cm}^3 \text{cm}^{-3}$). In particular, PTF4 showing a very good match between estimated and measured values, makes use of regression relationships simpler than those of PTF3 (**Table 3**). This can be considered a strength point for applicative purposes.

For PTF3 and PTF4, the influence of the pressure head on the soil water content estimations was also investigated by calculating the RMSD and AD values corresponding to pressure heads $h = -0.1, -1.0, -10.2$ and -153.0 m. For comparison, the same calculation was conducted for the PTF-MI since, among the literature PTFs, it provided the best results in terms of RMSD. For all considered pressure head values, lower RMSD values were obtained with specifically developed PTF3 and PTF4 than with PTF-MI (**Figure 3**). Moreover, in all cases, RMSD showed a clear decreasing trend with decreasing pressure head, suggesting an improvement in the accuracy of the estimation for lower values of soil water content (**Figure 3a**). A less reliable estimation of θ for

higher potentials is generally expected since, close to saturation, the water retention characteristic is mainly influenced by soil structure that does not directly figure in the considered PTFs (Tietje and Tapkenhinrichs 1993; Ungaro and Calzolari 2001). The water content was generally overestimated by PTF-MI and PTF3 as indicated by the AD values as a function of h (**Figure 3b**). In particular, PTF-MI tended to overestimate water content in the dry zone of the water retention curve and PTF3 in the wet one. PTF4 was characterized by lower distortions in the explored pressure head range and a clear dependence on the considered potential was not detected.

Validation of PTFs with independently measured water retention data obtained by the evaporation method showed relatively comparable performances for both recalibrated (PTF1 and PTF2) or specifically developed (PTF3 and PTF4) relationships. In particular, lower RMSD and AD values were detected for PTF1 and PTF3 (RMSD = 0.0421-0.0399 $\text{cm}^3 \text{cm}^{-3}$; AD = 0.0129-0.0220 $\text{cm}^3 \text{cm}^{-3}$) as compared with PTF2 and PTF4 (RMSD = 0.0524-0.0475 $\text{cm}^3 \text{cm}^{-3}$; AD = 0.0475-0.0260 $\text{cm}^3 \text{cm}^{-3}$), suggesting that a relatively more accurate and less biased estimation of θ can be obtained by either recalibrated or specifically developed PTFs. Measured and estimated water retention data were always significantly correlated (**Figure 4**), but the regression line did not coincide with identity one according to the 95% confidence intervals for the intercept, a , and the slope, b , of the regression line ($a \neq 0$ and $b = 1$ for PTF2 and PTF3, $a \neq 0$ and $b \neq 1$, for PTF1 and PTF4). This suggested that PTF2 and PTF3 tended to overestimate water retention data whereas PTF1 and PTF4 provided relatively small overestimation for low θ values and underestimation close to saturation. Moreover, although PTF1 and PTF3 were relatively more accurate than PTF2 and PTF4, they are not fully equivalent in terms of input variables, as PTF1 needs d_g and σ_g values which implies a detailed measurement of soil particle distribution. PTF3 requires only basic soil properties (i.e., Cl , Sa and OC) and thus offers a practical advantage for the not-specialized users. Overall, the RMSD values calculated for the validation data set were comparable, or even better, than those obtained with the calibration one thus confirming that the ENR technique is a valuable tool for

recalibrating/developing new PTFs for regions in which they are lacking. The evaporation method, allowing a fast determination of a high number of water retention data in the pressure head range relevant for water flow simulations, can be recommended as an alternative to classical equilibrium methods for PTFs validation.

Conclusions

The performance of eight existing PTFs were compared for a database of 217 water retention characteristics of Sicilian soils, covering a broad range of texture and land uses. Four alternative PTFs were also developed to estimate the parameters of van Genuchten model starting from easily determinable soil properties, such as texture and *OC*.

The results confirmed that application of PTFs to soils different from those used for their development can give rise to inaccurate estimates. Comparisons with independent soil data set are therefore recommended to avoid gross inaccuracies in the soil water retention estimation. A relatively better accuracy was obtained when PTF by Minasny et al. (1999) (PTF-MI) was applied, followed by PTF-HY or PTF-VE, PTF-S2, PTF-S1, PTF-RB, PTF-SC and PTF-ZW (RMSD range: 0.0630-0.0972 cm³ cm⁻³).

Application of ENR technique confirmed the potential in calibrating existing PTFs or developing new ones. Recalibrated PTF-MI and PTF-ZW relationships (respectively, PTF1 and PTF2) resulted in improved predictive performances. In particular, RMSD was improved by a factor 2 and AD by two orders of magnitude for PTF2. Specifically developed PTFs for Sicilian soils (PTF3 and PTF4), that require as input easily available information as texture and *OC*, resulted in RMSD values by 75-78% lower than those obtained by PTF-MI that scored as the best uncalibrated PTF for Sicilian soils. Organic carbon content was considered in the recalibrated/developed PTFs in place of ρ_b ; this choice can provide greater accuracy for agricultural soils, where undisturbed samples can be affected by errors due to compaction. Validation of recalibrated/developed PTFs for Sicilian soils, conducted by an independent data set obtained with the evaporation method, further corroborated

the reliability of the relationships proposed in this investigation. Comparable performances were observed for both recalibrated or specifically developed PTFs. However, PTF3 that yielded the lowest RMSD value, was preferred for estimating water retention of Sicilian soils as more parsimonious in terms of input data. Evaporation method was suitable for the experimental purposes and therefore may be recommended for an accurate validation of soil water retention PTFs. Future activities should be addressed to fill the gap in the knowledge of soil physical and hydraulic properties in Mediterranean areas. At the same time, there is the need to explore the potential of data mining techniques (i.e., neural regression, nearest neighbor or genetic algorithms) as indirect methods for predicting the soil hydraulic characteristics along with their uncertainties.

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Figure captions

Figure 1. USDA classification for the 217 soils considered in this investigation

Figure 2. Comparison between measured (θ_m) and corresponding predicted (θ_p) soil water contents using the considered PTFs.

Figure 3. Root mean squared differences (RMSD) and average differences (AD) calculated for each considered pressure head value, h .

Figure 4: Comparison between measured (evaporation method) and corresponding predicted soil water contents using recalibrated (PTF1 and PTF2) and developed (PTF3 and PTF4) pedotransfer functions for the selected Sicilian soils.

Table 1: Equations for the PTFs considered in the investigation.

Piecewise water retention models

PTF-S1 – Saxton et al. (1986)

$$\theta = \theta_s \text{ for } 0 < h \leq h_b$$

$$\theta = \theta_{10} + (\theta_s - \theta_{10}) \frac{(102 - h)}{(102 - h_b)} \text{ for } h_b < h \leq 102 \text{ cm}$$

$$\theta = \left(\frac{h}{10.2A} \right)^{1/B} \text{ for } h > 102 \text{ cm}$$

$$\text{with: } \theta_s = 0.332 - 7.251 \cdot 10^{-4} Sa + 0.1276 \log_{10}(Cl)$$

$$h_b = 1020 (-0.108 + 0.341 \theta_s)$$

$$\theta_{10} = \exp[(2.302 - \ln(A)) / B]$$

$$A = \exp[-4.396 - 0.0715Cl - 4.88 \cdot 10^{-4} Sa^2 - 4.285 \cdot 10^{-5} Sa^2 Cl] \cdot 100$$

$$B = -3.140 - 2.22 \cdot 10^{-3} Cl^2 - 3.484 \cdot 10^{-5} Sa^2 Cl$$

PTF-S2 – Saxton and Rawls (2006)

$$\theta = \theta_s \text{ for } 0 < h \leq h_b$$

$$\theta = \theta_{33} + (\theta_s - \theta_{33}) \frac{(336.6 - h)}{(336.6 - h_e)} \text{ for } h_b < h \leq 336.6 \text{ cm}$$

$$\theta = \left(\frac{h}{10.2A} \right)^{1/B} \text{ for } h_b > 336.6 \text{ cm}$$

$$\text{with: } A = \exp(\ln 33 + B \ln(\theta_{33}))$$

$$B = -3.817 / (\ln(\theta_{33}) - \ln(\theta_{1500}))$$

$$\theta_s = \theta_{33} + \theta_{s-33} - 9.7 \cdot 10^{-4} Sa + 0.043$$

$$\theta_{33} = 1.283(\theta_{33t})^2 + 0.626\theta_{33t} - 0.015$$

$$\theta_{33t} = -0.00251Sa + 0.00195Cl + 0.011OM + 6 \cdot 10^{-5} Sa \cdot OM - 0.000$$

$$\theta_{s-33} = 1.636\theta_{(s-33)t} - 0.107$$

$$\theta_{(s-33)t} = 0.00278Sa + 0.00034Cl + 0.022OM - 0.00018Sa \cdot OM - 0.$$

$$\theta_{1500} = 1.14\theta_{1500t} - 0.02$$

$$\theta_{1500t} = -0.00024Sa + 0.00487Cl + 0.006OM + 5 \cdot 10^{-5} Sa \cdot OM - 0.0$$

$$h_b = 10.2 \cdot [0.02(h_{bt})^2 + 0.887h_{bt} - 0.70]$$

$$h_{bt} = -0.2167Sa - 0.2793Cl - 81.97\theta_{s-33} + 0.7112Sa \cdot \theta_{s-33} + 0.0829Cl \cdot \theta$$

Brooks and Corey (1964) water retention model

$$\theta = \theta_s \text{ for } 0 < h \leq h_b$$

$$\theta = \theta_r + (\theta_s - \theta_r) (h_b / h)^\lambda \text{ for } h < h_b$$

PTF-RB – Rawls and Brakensiek (2006)

$$\theta_s = \Phi$$

$$\theta_r = -0.0182482 + 0.00087269Sa + 0.00513488Cl + 0.02939286\Phi - 0.00015395Cl^2 - 0.0010827Sa \cdot \Phi - 0.00018233Cl^2 \cdot \Phi^2 + 0.00030703Cl^2 \cdot \Phi - 0.$$

$$h_b = \exp(5.3396738 + 0.1845038Cl - 2.48394546\Phi - 0.00213853Cl^2 - 0.4356349Sa \cdot \Phi - 0.61745089Cl \cdot \Phi + 0.00143598Sa^2 \cdot \Phi^2 - 0.00855375Cl^2 \cdot \Phi^2 - 0.00072472Sa^2 \cdot \Phi + 0.0000054Cl^2 \cdot Sa + 0.50028060\Phi^2 \cdot Cl)$$

$$\lambda = \exp(-0.77842831 + 0.0177544Sa - 1.062498\Phi - 0.00005304Sa^2 - 0.00273493Cl^2 + 1.11134946\Phi^2 - 0.03088295Sa \cdot \Phi + 0.00026587Sa^2 \cdot \Phi^2 - 0.000798746Cl^2 \cdot \Phi - 0.00674491\Phi^2 \cdot Cl)$$

Table 1 (continue): Equations for the PTFs considered in the investigation.

van Genuchten (1980) water retention model

$$\theta = \theta_r + (\theta_s - \theta_r) \left(1 + |\alpha h|^n \right)^{-m} \quad m = 1 - 1/n \quad (m = -1 \text{ for PTF-VE})$$

PTF-HY – Wosten et al. (1999)

$$\theta_s = 0.7919 + 0.001691Cl - 0.29619\rho_b - 0.000001491Si^2 + 0.0000821OM^2 + 0.02427Cl^1 + 0.01113Si^{-1} + 0.01472\ln(Si) - 0.0000733OM \cdot Cl - 0.000619\rho_b \cdot Cl - 0.001183\rho_b \cdot OM - 0.0001664topsoil \cdot Si$$

$$\theta_r = 0$$

$$\alpha = \exp(-14.96 + 0.03135Cl + 0.0351Si + 0.646OM + 15.29\rho_b - 0.192topsoil - 4.671\rho_b^2 - 0.000781Cl^2 - 0.00687OM^2 + 0.0449OM^1 + 0.0663\ln(Si) + 0.1482\ln(OM) - 0.04546\rho_b \cdot Si - 0.4852\rho_b \cdot OM + 0.00673topsoil \cdot Cl)$$

$$n = 1 + \exp(-25.23 - 0.02195Cl + 0.0074Si - 0.1940OM + 45.5\rho_b - 7.24\rho_b^2 + 0.0003658Cl^2 + 0.002885OM^2 - 12.81\rho_b^{-1} - 0.1524Si^{-1} - 0.01958OM^1 - 0.2876\ln(Si) - 0.0709\ln(OM) - 44.6\ln(\rho_b) - 0.02264\rho_b \cdot Cl + 0.0896\rho_b \cdot OM + 0.00718topsoil \cdot Cl)$$

PTF-VE – Vereecken et al. (1989)

$$\theta_s = 0.81 - 0.283\rho_b + 0.001Cl$$

$$\theta_r = 0.015 + 0.005Cl + 0.014OC$$

$$\alpha = \exp(-2.486 + 0.025Sa - 0.351OC - 2.617\rho_b - 0.023Cl)$$

$$n = \exp(0.053 - 0.009Sa - 0.013Cl + 0.00015Sa^2)$$

PTF-SC – Scheinost et al. (1997)

$$\theta_s = 0.85 \phi + 0.13Cl$$

$$\theta_r = 0.51 Cl + 0.0017C_{org}$$

$$\alpha = (0.00023 + 0.007d_g)$$

$$n = 0.33 + 2.6 \sigma_g^{-1}$$

PTF-MI – Minasny et al. (1999)

$$\theta_s = 0.001 P_{<2} + 0.82607 \phi$$

$$\theta_r = -0.00733 + 0.00427 P_{<2} + 0.00267 P_{2-20}$$

$$\alpha = (0.1361 + 1.6929 d_g) \cdot 0.1$$

$$n = 1.4062 - 0.0050 \sigma_g$$

PTF-ZW – Zacharias & Wessolek (2007)

for $Sa < 66.5\%$

$$\theta_s = 0.0788 + 0.001 Cl - 0.263 \rho_b$$

$$\theta_r = 0$$

$$\ln(\alpha) = -0.648 + 0.023 Sa + 0.044 Cl - 3.168 \rho_b$$

$$n = 1.392 - 0.418 Sa^{-0.024} + 1.212 Cl^{-0.704}$$

PTF-ZW – Zacharias & Wessolek (2007)

for $Sa \geq 66.5\%$

$$\theta_s = 0.890 - 0.001 Cl - 0.322 \rho_b$$

$$\theta_r = 0$$

$$\ln(\alpha) = -4.197 + 0.013 Sa + 0.076 Cl - 0.276 \rho_b$$

$$n = -2.562 + 7 \times 10^{-9} Sa^{4.004} + 3.750 Cl^{-0.016}$$

Cl (%) clay; Si (%) silt; Sa (%) sand; Φ ($\text{cm}^3 \text{cm}^{-3}$) soil porosity; ρ_b (g cm^{-3}) soil bulk density; OM (%) organic matter content; OC (%) organic C content; C_{org} (g kg^{-1}) organic C content; $topsoil$ (-) qualitative variable having the value 1 (true) or 0 (false); θ_s ($\text{cm}^3 \text{cm}^{-3}$) saturated water content; θ_r ($\text{cm}^3 \text{cm}^{-3}$) residual water content; α (cm^{-1}), n and m parameters of water retention function by van Genuchten (1980); h_b (cm) and λ parameters of water retention function by Brooks and Corey (1964); $P_{<2}$, P_{2-20} and $P_{20-2000}$ mass of particles of ISSS classification $<2 \mu\text{m}$, $2-20 \mu\text{m}$ and $20-2000 \mu\text{m}$.

Table 2. Statistics of chemical and physical characteristics of the soils included in the considered database and measured soil water contents at selected pressure head values from -0.05 to -153 m.

<i>Variable</i>	<i>N</i>	<i>Min</i>	<i>Max</i>	<i>Mean</i>	<i>CV%</i>
<i>Cl</i> (%)	217	0.8	67.3	20.9	71.7
<i>Si</i> (%)	217	4.4	82.2	40.8	41.3
<i>Sa</i> (%)	217	0.05	91.8	38.3	59.2
<i>d_g</i> (mm)	216	0.001	0.129	0.027	94.6
σ_g (mm)	216	2.589	14.877	7.239	27.0
<i>OC</i> (g kg ⁻¹)	217	0.9	37.0	10.8	67.3
ρ_b (g cm ⁻³)	217	0.83	1.88	1.28	13.7
ϕ	217	0.29	0.69	0.51	12.5
$\theta_{-0.05}$	213	0.23	0.68	0.47	17.1
$\theta_{-0.1}$	216	0.23	0.68	0.45	17.2
$\theta_{-0.2}$	216	0.22	0.67	0.43	16.8
$\theta_{-0.4}$	217	0.20	0.67	0.40	18.2
$\theta_{-0.7}$	213	0.09	0.67	0.37	21.8
$\theta_{-1.0}$	102	0.08	0.47	0.32	23.8
$\theta_{-1.2}$	103	0.14	0.49	0.37	21.3
$\theta_{-1.5}$	35	0.19	0.39	0.30	15.5
$\theta_{-3.0}$	25	0.14	0.41	0.29	25.2
$\theta_{-3.37}$	169	0.03	0.48	0.31	32.7
$\theta_{-6.0}$	25	0.13	0.39	0.28	26.0
$\theta_{-10.2}$	213	0.05	0.41	0.24	33.3
$\theta_{-30.6}$	217	0.03	0.33	0.20	35.7
θ_{-153}	215	0.02	0.32	0.17	37.3

Table 3. Results of PTF application to Sicilian soils.

	RMSD	AD
	(cm ³ cm ⁻³)	(cm ³ cm ⁻³)
PTF-S1	0.0752	0.0037
PTF-S2	0.0727	0.0091
PTF-RB	0.0782	0.0021
PTF-HY	0.0680	-0.0106
PTF-VE	0.0680	-0.0108
PTF-SC	0.0939	0.0504
PTF-MI	0.0630	0.0070
PTF-ZW	0.0972	0.0618
PTF1	0.0594	-0.0017
PTF2	0.0508	0.0005
PTF3	0.0491	0.0092
PTF4	0.0470	0.0002

Table 4. PTFs developed with the database of Sicilian soils.

PTF1	PTF2
$\theta_s = 0.00171 \cdot Cl + 0.85646 \cdot \phi$	$\theta_s = 0.70751 + 0.00004 \cdot Cl - 0.17110 \cdot \rho_b$
$\theta_r = -0.03966 + 0.00217 \cdot Cl + 0.00384 \cdot Si$	$\theta_r = 0$
$\alpha = 0.02994 + 0.23924 \cdot d_g$	$\ln \alpha = -3.16238 + 0.02841 \cdot Cl + 0.06349 \cdot Sa - 2.15479 \cdot \rho_b$
$n = 1.44633 - 0.00792 \cdot \sigma_g$	$n = -8.42482 + 6.13905 \cdot Cl^{-0.0007} + 3.40920 \cdot Sa^{-0.0049}$
PTF3	PTF4
$\theta_s = 0.44517 + 0.00029 \cdot Cl + 0.00445 \cdot OC$	$\theta_s = 0.44048 + 0.00035 \cdot Cl + 0.00451 \cdot OC$
$\theta_r = 0$	$\theta_r = 0$
$\ln \alpha = -5.80454 + 0.02925 \cdot Cl + 0.05670 \cdot Sa + 0.1057 \cdot OC$	$\ln \alpha = -1.16757 - 0.03413 \cdot Si$
$n = -13.72698 + 9.68542 \cdot Cl^{-0.0012} + 5.18344 \cdot Sa^{0.0033}$	$n = 1.08512 + 0.00188 \cdot Sa + 0.00051 \cdot OC$

Dependent variables: Cl (%) clay; Si (%) silt; Sa (%) sand; ϕ ($\text{cm}^3\text{cm}^{-3}$) porosity; ρ_b (g cm^{-3}) dry bulk density; OC (%) organic carbon content; d_g (mm) and σ_g (mm) geometric mean and geometric standard deviation of mean diameter of soil particles.

Independent variables: θ_r ($\text{cm}^3\text{cm}^{-3}$) residual water content, θ_s ($\text{cm}^3\text{cm}^{-3}$) saturated water content, α (cm^{-1}) scale parameter, n (-) shape parameter.

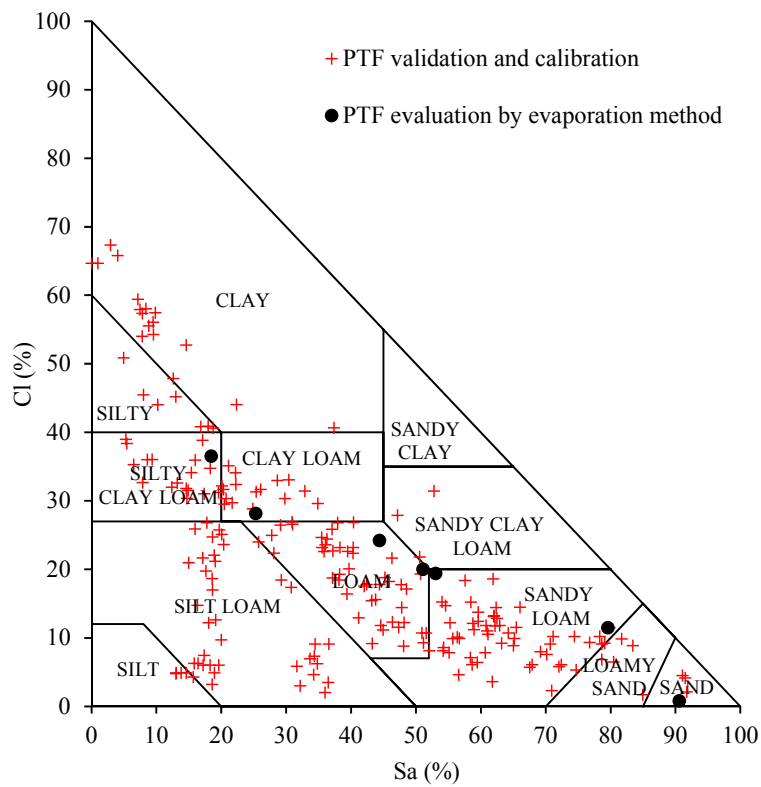


Figure 1. USDA classification for the 217 soils considered in this investigation

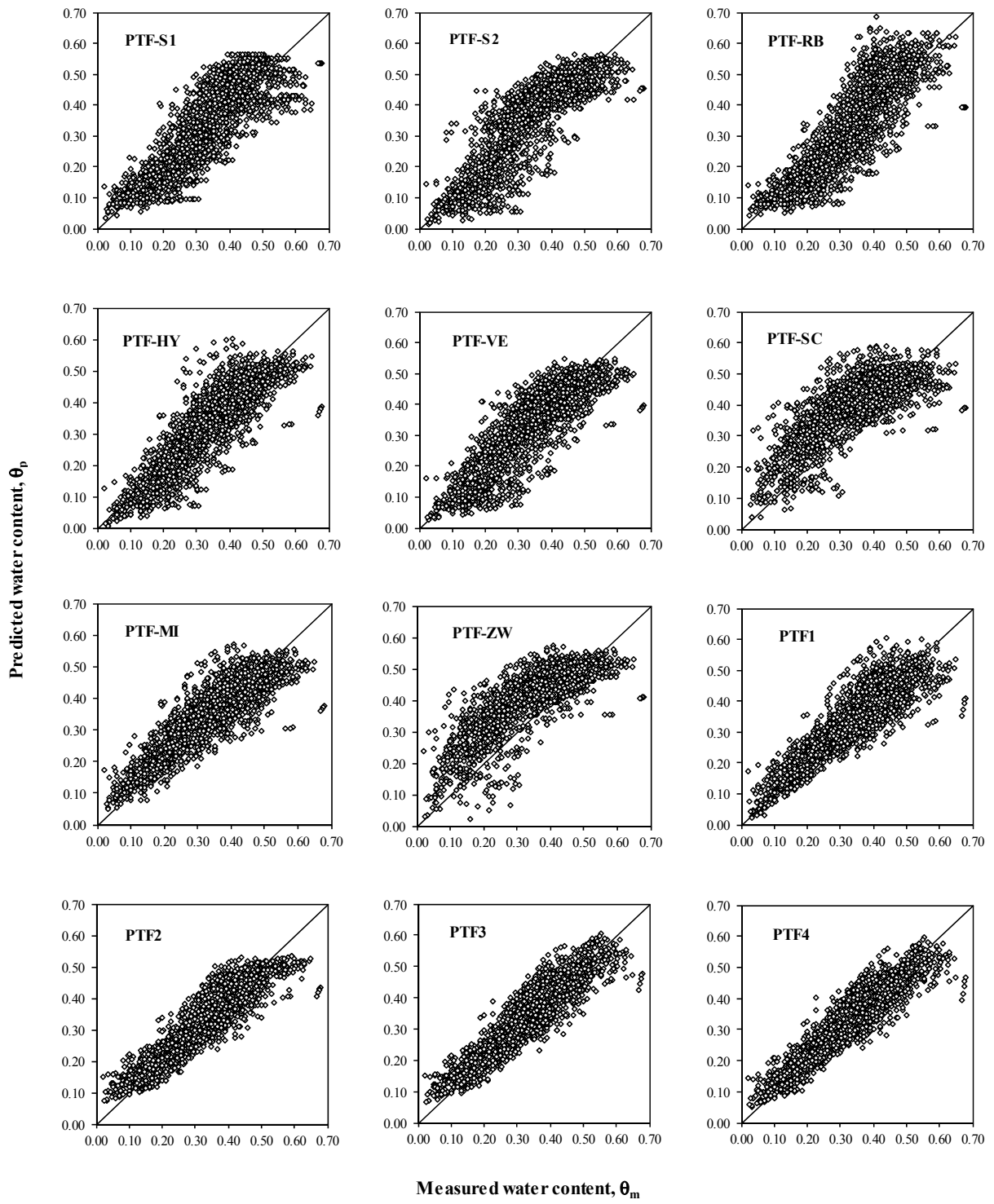


Figure 2.

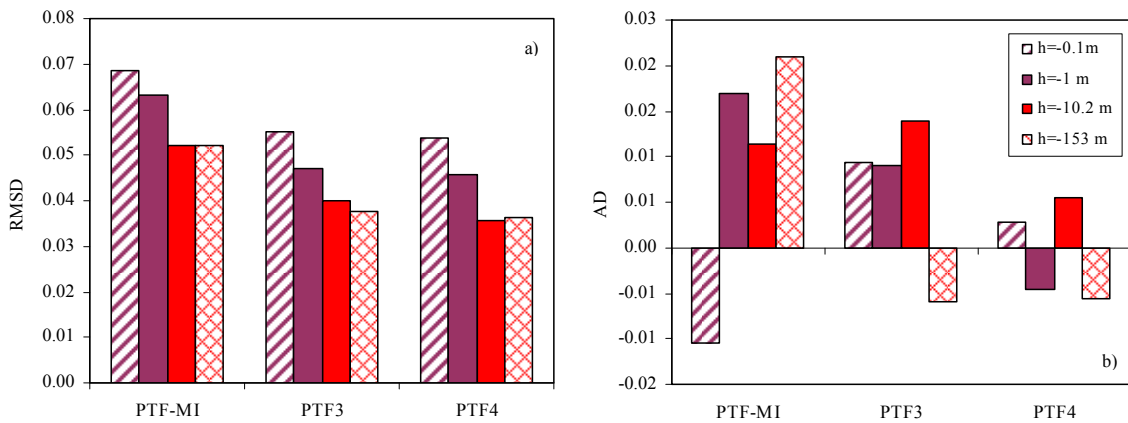
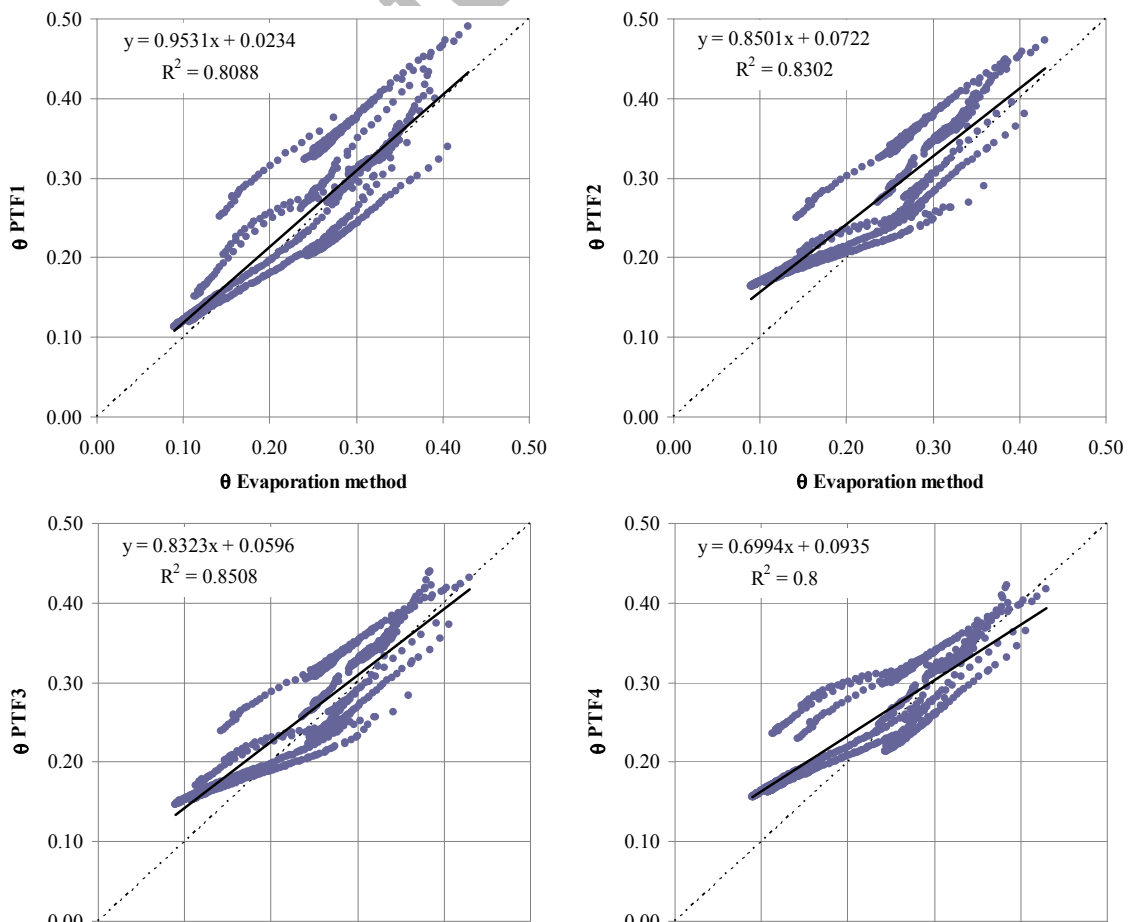


Figure 3.



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Figure 4.