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Prediction of saturated hydraulic conductivity Ks of agricultural soil using pedotransfer functions

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Abstract: The determination of the saturated hydraulic conductivity Ks on a field scale presents a challenge in which several variables have to be considered. As there is no benchmark or reference method for the Ks determination, the suitability of each available method has to be evaluated. This study is aimed at the functional evaluation of three publicly available types of pedotransfer functions (PTFs) with different levels of utilised predictors. In total, ten PTF models were applied to the 56 data sets including the measured Ks value and the required predictors (% sand, silt and clay particles, dry bulk density, and organic matter/organic carbon content). A single agricultural field with a relatively homogenous particle size distribution was selected for the study to evaluate the ability of the PTF to reflect the variability of Ks. The correlation coefficient, coefficient of determination, mean error, and root mean square error were determined to evaluate the Ks prediction quality. The results showed a high variability in Ks within the field; the measured Ks values ranged between 10 and 1261 cm/day. Although the tested PTF models are based on a robust background of soil databases, they could not provide estimates with satisfactory accuracy unless local soil data were incorporated into the PTF development.

Keywords: functional evaluation; machine learning; neural network, non-linear regression; soil hydraulic properties

Agricultural soils are subjected to the cultivation and fertilisation of the soil surface layer which results in changes to the soil hydrophysical properties. Plant growth and root development together with the activity of soil fauna result in a relatively high variation in the hydraulic properties of agricultural soils. In addition to that, the drying of the soil and the creation of cracks contribute to the formation of preferential pathways, allowing faster water infiltration and reaching deeper soil layers (Štekauerová & Mikulec 2009). Undesirable significant herbicide or pesticide contents can be leached from the surface to the deeper layers and/or to the groundwater (Fait et al. 2010; Willkommen et al. 2021). One of the most important hydraulic properties of each soil is the saturated hydraulic conductivity Ks. It is a widely used characteristic in soil water and solute transport models incorporated in a number of different environmental, hydrological and water management applications (Schaap et al. 2001; Araya & Ghezzehei 2019; Tuffour et al. 2019). Under most field conditions, soils are not only heterogeneous, but also anisotropic.

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The heterogeneity of the soil can be defined by the spatial variability of its properties, e.g., Ks. Anisotropy, on the other hand, leads to different property exhibitions in different directions; measured Ks values in the vertical direction may be higher or lower than those measured in the horizontal direction. There are several methods for the Ks measurement; in the field and in the laboratory by using different types of infiltrometers. Ks *in-situ* can be determined by, e.g., the Double-ring infiltrometer (Parr & Bertrand 1960), Hood infiltrometer (Schwärzel & Punzel 2007), Guelph infiltrometer (Soilmoisture Equipment Corp., USA), and SATURO (METER Group Inc., USA). Ks in the laboratory can be determined by a constant or falling head apparatus such as a K_{SAT} device (METER Group Inc.). Unfortunately, there is no standard procedure for the Ks determination, to which the others can be related to or compared with. Direct measurement can involve an unreasonably high number of replications to account for the spatial variability of Ks, especially when large and/or heterogeneous areas are being characterised. That is why indirect Ks estimation methods of have been developed. Bouma and van Lanen (1987) introduced the term "transfer functions" and later Bouma (1989) introduced the term "pedotransfer functions (PTFs)" for these estimation methods. Minasny et al. (1999) described PTF as a translation of data "we have" into data "we need". Ks estimations are based on routinely measured and easily available soil properties called predictors, such as the particle size distribution data, dry bulk density, and organic matter/organic carbon content. Over the last 30 years, numerous PTFs have been proposed and their estimation quality has been evaluated and compared mainly for the prediction of soil water retention parameters; however, a review by Zhang and Shaap (2019) provided an insight into the history of Ks predictions, and discussed the required predictors and statistical techniques for the PTF development.

There are many types and forms of PTF; PTF can be grouped according to some basic criteria. Wösten et al. (1998) divided the PTF into two groups: Class PTF attributing the values of Ks according to their relevance to a particular soil texture class and, Continuous PTF where linear, reciprocal and exponential relationships of the predictors were used in the regression analysis. Tomasella et al. (2003) divided the empirical PTF into two other groups: Point PTF and Parametric PTF. Minasny et al. (1999) presented parametric and point estimates based on multiple linear regression, extended non-linear regression and artificial neural networks (NNs). NN analysis is implemented in a user-friendly program Rosetta, where Schaap et al. (2001) used a hierarchical approach to estimate Ks for different levels of the available predictors. Kröse and van der Smagt (1996) described NN as a highly interconnected network created by simple processing units (neurons) which communicate by sending signals to each other over the weighted connections. Each unit receives input from external sources, computes an output signal from it and propagates it to the other units. Three types of units (layers) are usually distinguished: input units which receive data from outside the neural network, output units which send the data out of the neural network and hidden units which are between the input and output units (their input and output signals remain within the neural network).

The recent technical progress in high-performance computing together with a collection of soil hydraulic data into large databases has enabled the development of data-driven methods such as machine learning technique (ML). PTF for Ks prediction using four types of ML-algorithms were published by Araya and Ghezzehei (2019); models using the K-Nearest Neighbours, Support Vector Regression, Random Forest (RF) and Boosted Regression Trees (BRTs) for different levels of predictors are available within their PTF App. The RF method averages the decisions of the large number of individually grown decision trees by searching for a predictor that provides the best split, resulting in the smallest model error. Gunarathna et al. (2019) reported this method as relatively robust to errors and outliers. BRT combines two algorithms: Regression Trees relating the response to their predictors by recursive binary splits and an adaptive method for combining many simple models for the improvement of the predictive performance called boosting (Elith et al. 2008). Thanks to their operating principle, BRT-based PTF are attractive in works with different origins of the training data, such as Ks measurement *in-situ*/laboratory by different methods (Araya & Ghezzehei 2019). The BRT and RF methods incorporated within the PTF App are based on more than 18 000 datasets of United States (US) soils and offer predictions based on up to 20 predictors. Such a large background database might imply the possibility of use for the Ks estimation of soils outside the US.

This study aims to find out whether the Ks of an agricultural field with relatively high spatial and temporal variability in Ks can be estimated with acceptable accuracy by means of PTF based on different approaches;

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Table 1. Basic soil characteristics of the experimental site in Praha-Ruzyně

	OM	C_{ox}	Dry bulk density (g/cm^3)	Clay	Silt	Sand	Particle density (g/cm^3)	Ks (cm/day)
	(%)			(%)				
Min	1.241	0.720	1.13	22.0	54.2	8.0	2.60	10.2
Max	3.362	1.950	1.62	33.5	65.5	19.0	2.64	1 261.2
Average	2.339	1.357	1.35	30.2	57.2	12.6	2.62	336.8
SD	0.476	0.276	0.12	3.3	3.3	2.7	0.02	271.4

OM – organic matter content; C_{ox} – organic carbon content; SD – standard deviation; Ks – saturated hydraulic conductivity

NN analysis in Rosetta by Schaap et al. (2001), ML-algorithms in the PTF App by Araya and Ghezzehei (2019) and the continuous PTF by Wösten et al. (1998).

MATERIAL AND METHODS

Source data. This study utilised information about the particle size distribution (% clay, silt and sand), dry bulk density (BD) and organic matter (OM)/organic carbon (C_{ox}) paired with 56 Ks measurements. The Ks measurements were carried out *in situ* by a Pressure ring infiltrometer (Matula & Kozáková 1997) in 2008–2009 and also by a K_{SAT} device (METER Group, Inc.) in the laboratory on 250 cm^3 soil core samples in 2021. All the data originate from one agricultural field managed by different tillage operations since 1995 within the experimental research at the Crop Research Institute in Prague (altitude 345 m a.s.l., 50°5'17.264''N, 14°17'50.024''E, with a mean annual precipitation of 473 mm and a mean annual temperature of 7.9 °C). The following tillage treatments were repeatedly applied within the experimental field: conventional tillage with mouldboard ploughing up to 22 cm, reduced tillage with a non-inversion treatment of the top 10 cm by a chisel plough and no-tillage (direct drill). The following crop rotation is being used: pea (*Pisum sativum*) – winter wheat (*Triticum aestivum*) – oil seed rape (*Brassica napus* subsp. *napus*) – winter wheat (*Triticum aestivum*). The Ks data originate from measurements in all three types of crops in different phases of the vegetation season. The soil texture (Soil Survey Staff 2014) of the experimental field is silty clay loam (38 samples) and silt loam (18 samples) and the soil was classified as Haplic Luvisol (IUSS Working Group 2015), formerly referred to as Orthic Luvisol (FAO-UNESCO 1974). The basic soil properties (Table 1) were determined by standard methods; particle size distribution analysis by the Hydrometer Method, particle density by the Pycnometer Bottle Method, the dry bulk density (gravimetric method on 100 and/or 250 cm^3 undisturbed soil samples), the organic carbon content C_{ox} by the Walkley–Black oxidometric method (organic matter content was obtained by multiplication by a factor of 1.724).

Tested PTFs. Ten PTF models with different levels of predictors were evaluated in this study (Table 2). Two ML-algorithms with three levels of predictors

Table 2. List of the applied pedotransfer functions (PTF) and corresponding predictors

PTF model	Method	Predictors	Reference
BRT 3-0	boosted regression trees	% sand, % silt, % clay	Araya and Ghezzehei (2019)
BRT 3-1	boosted regression trees	% sand, % silt, % clay, BD (g/cm^3)	Araya and Ghezzehei (2019)
BRT 3-2	boosted regression trees	% sand, % silt, % clay, BD (g/cm^3), C_{ox} (%)	Araya and Ghezzehei (2019)
RF 3-0	random forest	% sand, % silt, % clay	Araya and Ghezzehei (2019)
RF 3-1	random forest	% sand, % silt, % clay, BD (g/cm^3)	Araya and Ghezzehei (2019)
RF 3-2	random forest	% sand, % silt, % clay, BD (g/cm^3), C_{ox} (%)	Araya and Ghezzehei (2019)
Rosetta-SSC	neural network	% sand, % silt, % clay	Schaap et al. (2001)
Rosetta-SSC+BD	neural network	% sand, % silt, % clay, BD (g/cm^3)	Schaap et al. (2001)
Wösten-original p.	non-linear regression analysis	% silt, % clay, OM (%), BD (g/cm^3), topsoil	Wösten et al. (1998)
Wösten-own p.	non-linear regression analysis	% silt, % clay, OM (%), BD (g/cm^3), topsoil	Wösten et al. (1998)

BD – dry bulk density; C_{ox} – organic carbon content; OM – organic matter content; topsoil is a qualitative variable with a value of 1 for topsoil and 0 for subsoil

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from the ML-based PTF of Araya and Ghezzehei (2019) were selected for testing in this study: Random Forest (RF) and Boosted Regression Trees (BRTs). The NN analysis incorporated into the public domain Windows-based modelling program Rosetta (Schaap et al. 2001) offers a total of five hierarchical models of PTF, two of which were tested in this study. The continuous PTF of Wösten et al. (1998) was applied in its original form of Equation (1) and also with newly derived regression parameters (Equation (2)) specific for the silty clay loam texture class based on the soil water retention data contained in the database of soil hydrophysical properties in the Czech Republic (HYPRESCZ database) (Miháliková et al. 2013).

$$Ks^* = 7.755 + 0.0352 \times S + 0.93 \times topsoil - 0.967 \times D^2 - 0.000484 \times C^2 - 0.000322 \times S^2 + 0.001 \times S^{-1} - 0.0748 \times OM^{-1} - 0.643 \times \ln(S) - 0.01398 \times D \times C - 0.1673 \times D \times OM + 0.02986 \times topsoil \times C - 0.03305 \times topsoil \times S \quad (1)$$

$$Ks^* = 3149.75 + 26.33 \times S + 1.447 \times D^2 + 0.0023 \times C^2 - 0.1056 \times S^2 - 12119.6 \times S^{-1} - 0.0033 \times OM^{-1} - 1011.6 \times \ln(S) - 0.112 \times D \times C + 0.0911 \times D \times OM \quad (2)$$

where:
Ks* – transformed parameter Ks, Ks* = ln(Ks);
ln – a natural logarithm;
C – content of the clay particles (%);
D – dry bulk density (g/cm^3);
S – content of the silt particles (%);
OM – organic matter content (%).

Topsoil is a qualitative variable with a value of 1 for topsoil and 0 for subsoil.

Statistical evaluation. The quality of the Ks estimates was evaluated by the mean error (ME), the root mean square error (RMSE), the correlation coefficient (*r*), and the coefficient of determination (R^2), as follows:

$$\mathrm{ME} = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - x_i\right) \quad (3)$$

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(x_i - y_i\right)^2} \quad (4)$$

$$R^2 = \left\{\frac{n\sum_{i=1}^{n}x_i y_i - \sum_{i=1}^{n}x_i \sum_{i=1}^{n}y_i}{\sqrt{\left[n\sum_{i=1}^{n}x_i^2 - \left(\sum_{i=1}^{n}x_i\right)^2\right]\left[n\sum_{i=1}^{n}y_i^2 - \left(\sum_{i=1}^{n}y_i\right)^2\right]}}\right\}^2 \quad (5)$$

where:
x_i – measured Ks data;
y_i – predicted Ks data;
n – the number of x_i y_i data pairs.

For the possibility of comparison to other published studies, the Ks values were determined in cm/day. Since the Ks is not normally distributed, the statistical evaluation was performed on the log-transformed Ks data.

RESULTS AND DISCUSSION

In total, 56 Ks values were predicted by ten PTF models for a single agricultural field where different tillage practices have been applied repeatedly since 1995. The particle size distribution data, the essential predictors of each PTF, did not significantly differ in space and time. The maximum differences in % content of the clay, silt and sand particles reached

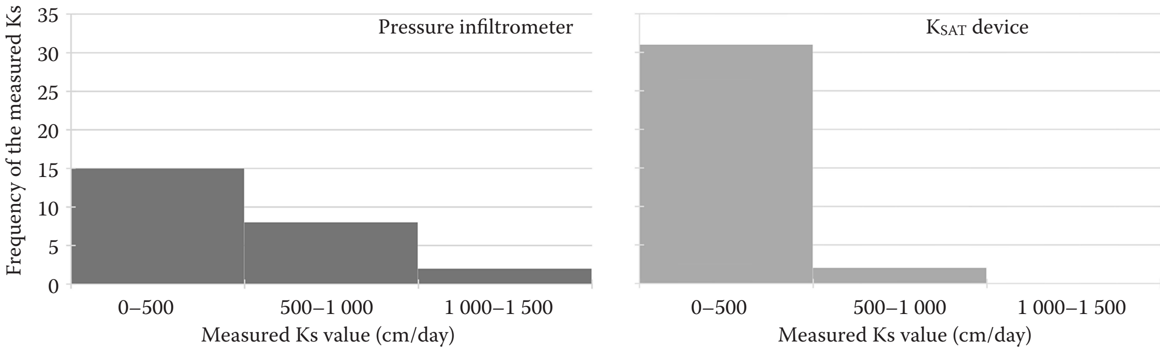

Figure 1. Frequency histograms of the measured saturated hydraulic conductivity (Ks) data; *in-situ* measurements utilising a Pressure infiltrometer by Matula and Kozáková (1997) on the left and laboratory measurements on 250 cm^3 undisturbed soil samples by a K_{SAT} device (METER Group Inc.) on the right

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Table 3. Statistical evaluation and final ranking of the tested pedotransfer functions (PTF) on the basis of the root mean square error (RMSE)

PTF model	*r*	R^2 (%)	ME	RMSE	Ranking*
Wösten-own p.	–0.038	0.147	–0.101	0.521	1
Rosetta SSC+BD	–0.076	0.584	–1.014	1.235	2
RF 3-0	0.008	0.006	–1.054	1.238	3
Wösten-original p.	0.253	6.393	–1.205	1.273	4
BRT 3-2	–0.094	0.881	–1.183	1.314	5
Rosetta SSC	0.232	5.390	–1.282	1.348	6
BRT 3-0	–0.138	1.912	–0.700	1.385	7
RF 3-2	0.101	1.020	–1.390	1.456	8
BRT 3-1	–0.071	0.508	–1.395	1.537	9
RF 3-1	0.095	0.907	–1.616	1.682	10

r – correlation coefficient; R^2 – coefficient of determination; ME – mean error; *the best ranking (1) is attributed to the PTF with the smallest RMSE value

11%, but the measured Ks value ranged from 10.2 cm/day to 1261.2 cm/day (Table 1). Such variability in Ks is common for agricultural fields, where tillage operations temporarily affect the soil structure (Šteakauerová & Mikulec 2009; Schwen et al. 2011). Smaller Ks values were measured on the undisturbed soil samples by the K_{SAT} device in the laboratory compared to the Ks values measured in the field (Figure 1). This might be due to the disturbance of the continuity of the porous system during the sampling and/or transportation process. Since there is no reference method for Ks determination, the possible effect of the determination method has not been evaluated and all the measured data were used for a quality evaluation of the Ks estimates. The resulting statistics ME, *r*, R^2 and RMSE are presented in Table 3, where the individual PTF models are ranked (1–10) according to their performance. The best ranking (1) was attributed to the PTF with the smallest RMSE value. The distribution of the measured and estimated Ks values in terms of quartiles is depicted in Figure 2; a very wide range of estimated Ks values was obtained from BRT 3-0. The individual estimates were checked and it was found that only a 2% difference in the clay or silt content resulted in estimates being two orders of magnitude different. An increase in the clay content from 30.6% to 32.6% with an unchanging silt content of 55.5% and a corresponding 2% decrease in the sand content from 13.9% to 11.9% caused a decrease in the estimated Ks value from 1573.8 to 10.5 cm/day. Similar to that, an increase in the silt content by 2% (from 55.5% to 57.5%, with an unchanged clay content of 30.6% and a corresponding 2% decrease in the sand content from 13.9% to 11.9%) also caused a significant drop in the estimated Ks value (from 1573.8 to 13.9 cm

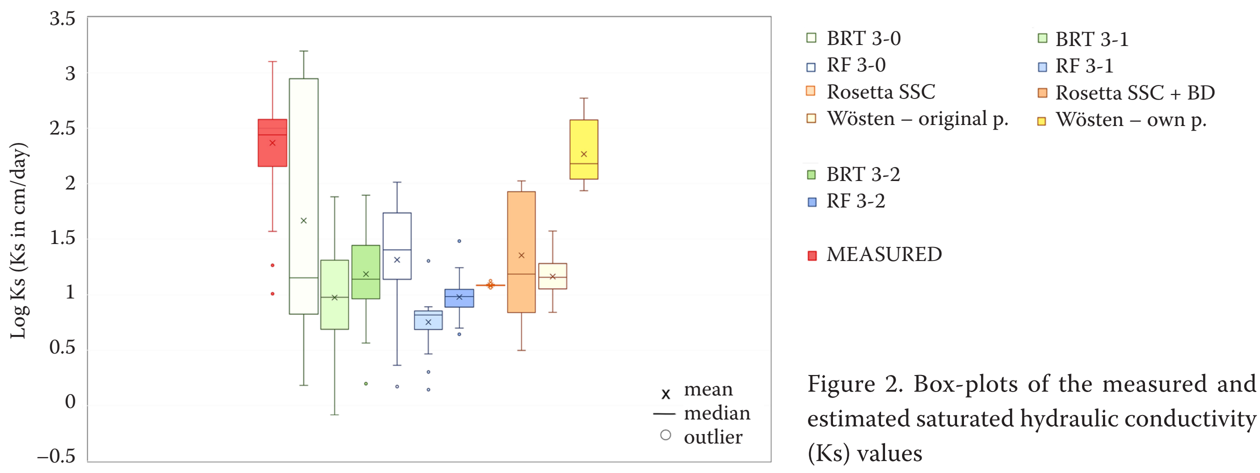

Figure 2. Box-plots of the measured and estimated saturated hydraulic conductivity (Ks) values

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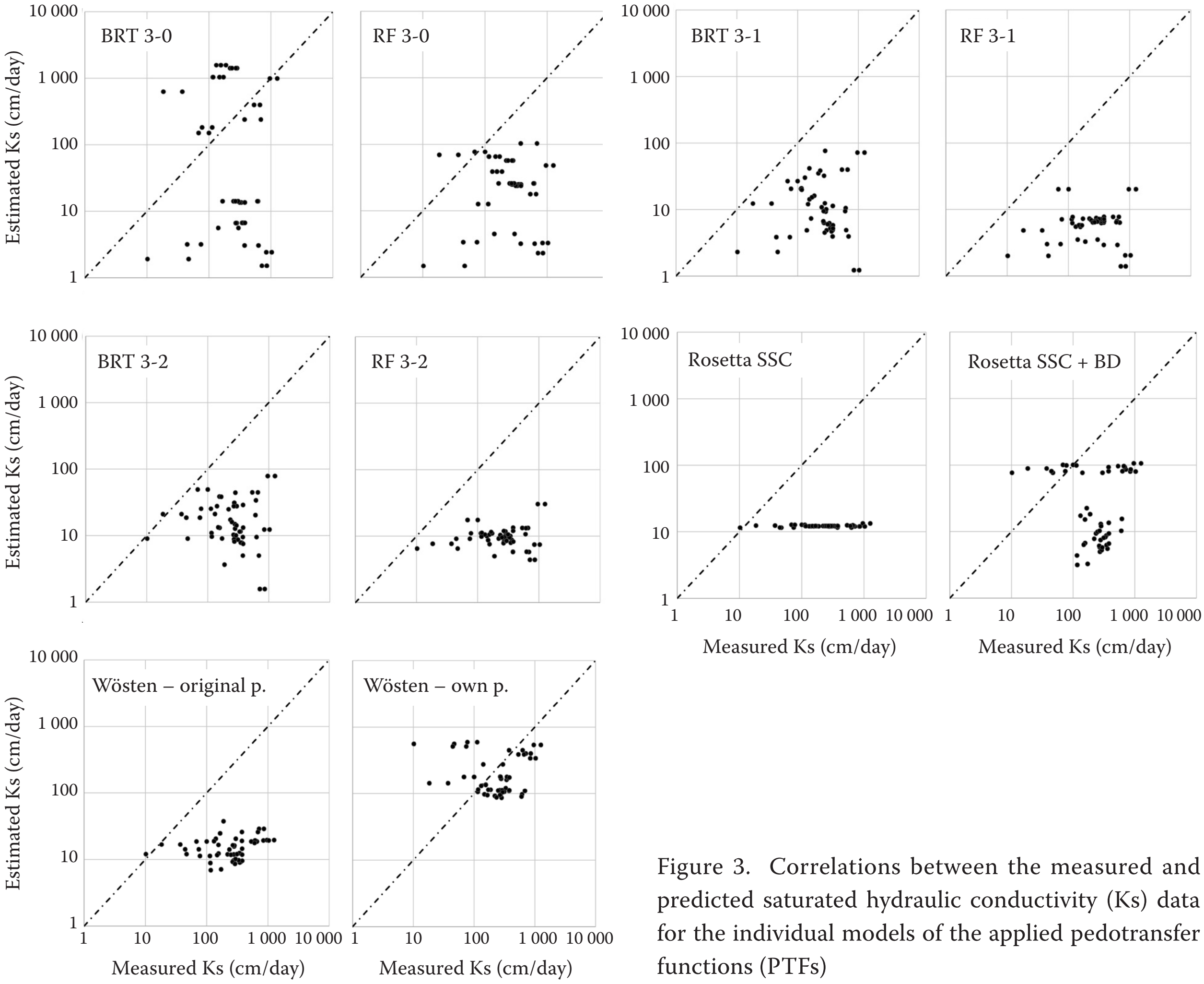

Figure 3. Correlations between the measured and predicted saturated hydraulic conductivity (Ks) data for the individual models of the applied pedotransfer functions (PTFs)

per day). These unreasonably high Ks estimates which appeared in 12 cases affected the BRT 3-0 performance, as documented by the correlation graphs displayed in Figure 3. Other BRT models with a higher number of predictors using not only the particle size distribution data, but also the BD (BRT 3-1) or BD and C_{ox} (BRT 3-2) did not show such an effect. Despite the above discussed cases of overestimations, from a general point of view, all the tested PTF models underestimated the measured data. The extent of the underestimation can be observed in Figure 4, where the resulting negative ME values are graphically displayed. Temporary enhanced infiltration caused by tillage operations (e.g., Moret & Arrúe 2007; Kreiselmeier et al. 2020) and/or higher pore connectivity and the macroporous preferential flow reported for no-tillage (reported by, e.g., Galdos et al. 2019) were not sufficiently reflected by the PTF.

The correlation between the measured and predicted Ks data is indicated by the r and R^2 coefficients; the higher the coefficients, the better the correlation. As can be seen from Table 3 and Figure 3, the correlation between the measured and estimated data is low. However, for some estimates, the low values of the r or R^2 coefficients do not necessarily mean a low estimation quality. Instead, the average deviation of the predicted Ks value from the measured Ks expressed as RMSE is considered as the most suitable characteristic for the evaluation of the Ks estimation quality. The lowest RMSE value of 0.521 was determined for the continuous PTF in a form by Wösten et al. (1998), for which the own regression parameters were derived based on the Czech database of soil hydraulic properties HYPRES CZ (Miháliková et al. 2013). This is the only PTF model which provided estimates of Ks for a given agricultural soil with acceptable accuracy comparable to other published studies (RMSE < 1). This is agreement with findings of Nemes et al. (2003) highlighting the need for national scale datasets to be utilised

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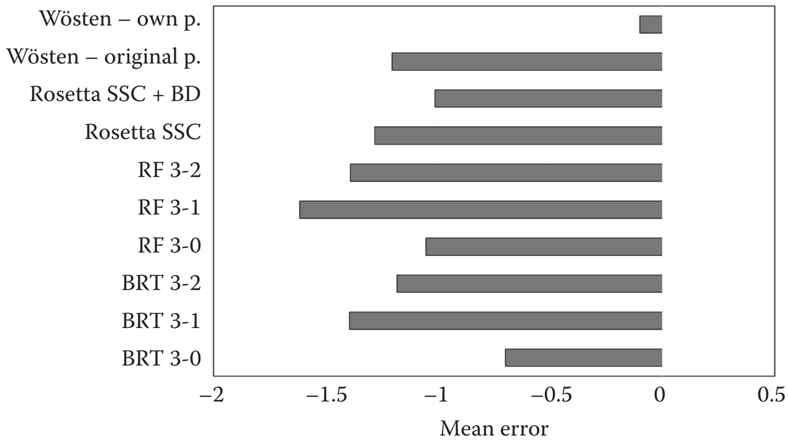

Figure 4. Estimation quality of the tested models of the pedotransfer functions (PTFs) by means of the mean error (ME)
The ME values are based on the log-transformed saturated hydraulic conductivity (Ks) values in cm/day

within the estimation procedures by PTF. Lilly et al. (2008) reported averaged RMSE values of 0.97 for PTF using Regression Trees and Tóth et al. (2015) reported RMSE for estimates on a European scale in a range from 0.9 to 1.36. Araya and Ghezzehei (2019) presented RMSE values between 0.34 and 0.44 for the BRT models and from 0.37 to 0.44 for models employing RF. Although a very robust soil database of more than 18 000 datasets is behind their PTF App, the individual texture classes are not uniformly represented; soils with coarse texture predominate within the database. The possible improvement in the estimation quality by means of incorporation of the local soil data into the ML-based PTF by Araya and Ghezzehei (2019) is planned for future studies. Estimations with other parameters reflecting changes in the soil properties caused by agrotechnical operations, such as aggregate stability is also planned to be explored.

CONCLUSION

Despite the large databases behind the PTF in Rosetta (Schaap et al. 2001) and the PTF App (Araya & Ghezzehei 2019), these PTF did not provide satisfactory estimates for the agricultural soil being investigated (Haplic Luvisol, in the Czech Republic). The soil reflects changes in the structure due to tillage operations and, thus, has a great temporal variability, which is difficult to describe by predictors. The importance of local, national-based databases of soil hydraulic properties has been confirmed as they can provide background data which can lead to higher quality estimates of Ks. Although the use of estimated saturated hydraulic conductivity values is becoming more common, the importance of direct determination methods should not be downplayed.

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