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Hydrophysical properties of irrigated and irrigable soils with regards to their ongoing degradation

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Doctoral Dissertation

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Prague 2 0 2 3

DECLARATION

I declare that I have written my Ph.D. thesis aimed at "Hydrophysical properties of irrigated and irrigable soils with regards to their ongoing degradation" independently under the guidance of my supervisor, **prof. Ing. Svatopluk Matula, CSc.** and co-supervisor **Ing. Markéta Miháliková, Ph.D.** I have used the literature and other information sources that are cited in the work and listed in references attached at the end of this work. As the author of the thesis, I declare that I am responsible for its creation and did not trespass the copyright of the third parties.

Prague, November 14, 2023

Signature

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PREFACE

The thesis presented herein comprises a collection of publications spanning the years 2019 to 2023. This collection has been organized into distinct sections and interconnected based on the objectives and the scientific hypotheses they aimed to explore. The methodological approaches and findings detailed in this thesis adhere closely to established scientific protocols. The research methodologies employ comprehensive approaches tailored to each study's requirements. The focus of this thesis revolves around the essential domain of soil hydrology, encompassing diverse aspects such as hydraulic conductivity, field capacity estimation, and the effects of surfactants on soil properties. The research draws upon a rich array of datasets from various sources, integrating fieldwork, laboratory experiments, and advanced statistical evaluations to derive meaningful conclusions. The oversight and guidance provided by the Department of Water Resources at the Czech University of Life Sciences Prague, have been instrumental in shaping and steering this body of work. As we proceed on this journey, we anticipate that this work will contribute to long-term environmental sustainability and more effective soil and water management across diverse environmental contexts.

Below are the publications that constitute the thesis:

Almaz, C., Kara, R. S., Miháliková, M., & Matula, S. (2023). Implications of surfactant application on soil hydrology, macronutrients, and organic carbon fractions: An integrative field study. *Soil and Water Research 18(4*), 269-280. https://doi.org/10.17221/88/2023-SWR

Almaz, C., Miháliková, M., Báťková, K., Vopravil, J., Matula, S., Khel, T., & Kara, R. S. (2023). Simple and Cost-Effective Method for Reliable Indirect Determination of Field Capacity. *Hydrology, 10(10)*, 202. https://doi.org/10.3390/hydrology10100202

Batkova, K., Matula, S., Hrúzová, E., Miháliková, M., Kara, R. S., & Almaz, C. (2022). A comparison of measured and estimated saturated hydraulic conductivity of various soils in the Czech Republic. *Plant, Soil and Environment*, *68*(7), 338-346. https://doi.org/10.17221/123/2022-PSE

Báťková, K., Matula, S., Miháliková, M., Hrúzová, E., Abebrese, D. K., Kara, R. S., & Almaz, C. (2023). Prediction of saturated hydraulic conductivity Ks of agricultural soil using pedotransfer functions. *Soil & Water Research*, *18*(1). https://doi.org/10.17221/130/2022-SWR

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1. Literature Review

1.1. Introduction to Hydrophysical Properties of Soils and their Degradation

Soil degradation is a pressing global issue in the 21st century due to population growth, land use pressure, and climate change. Approximately 33% of the Earth's surface has been affected by accelerated soil degradation (Bini, 2009; Monanarella et al., 2015; Hossain et al., 2020), leading to reduced soil quality and ecosystem functions (Lal, 2015a; Lal, 2009a). The world's land resources are finite and fragile, with only about 22% suitable for cultivation and 3% having high agricultural production capacity (Lal, 1997; Lal, 2009b). Official reports highlight the imminent threat of soil degradation (European Environment Agency, 2000). Researchers underscore the global significance of agricultural land degradation, affirming its enduring prominence on the international agenda from the twentieth century into the twenty-first century (Utuk and Daniel, 2015). Soil degradation manifests through processes like erosion, loss of organic matter, compaction, acidification, and contamination (Jie et al., 2002; Nouwakpo et al., 2018; Zhang, 2020), significantly impacting agricultural sustainability (Scherr, 1999; Lal, 2015a; Chalise et al., 2019; Zhang, 2020).

Soil erosion, a prominent factor in degradation (Bonthagorla et al., 2022), encompasses both wind and water erosion. It involves the exfoliation, dispersion, and destruction of surface materials under the influence of external forces such as hydraulic power, wind, and gravity (Noori et al., 2018). Specifically, water erosion affects around 115 million hectares, constituting 12% of the total land area, while wind erosion impacts 42 million hectares, with 2% experiencing significant erosion (European Environment Agency, 2015; Bednář and Šarapatka, 2018). Approximately 40% of agricultural land is undergoing severe degradation, with water erosion emerging as a major threat in Europe (Boardman and Poesen, 2006). Projecting forward to 2050, there is a potential increase in mean soil loss rates due to water erosion by 13–22.5% in agricultural areas of both the EU and the UK, as compared to the baseline in 2016 (Panagos et al., 2021). The Czech Republic faces a substantial challenge, with over 50% of its agricultural land under threat from water erosion (Ministry of Agriculture of the CR, 2015). The European Union emphasizes erosion due to its substantial impact on food production, water resources, biodiversity, ecosystems, and carbon stocks (Lal, 2005; Boardman and Poesen, 2006).

Wind erosion affects around 14.31% of agricultural land in the Czech Republic, particularly in drier regions with specific soil types (Šarapatka, and Bednář, 2015). Soil compaction, primarily induced by heavy machinery and intensified by intensive tillage practices (Hossain et al., 2020), affects almost half of the agricultural land in the Czech Republic (Ministry of Agriculture of the CR, 2012), impacting water infiltration, reducing porosity, root growth, nutrient uptake and increasing surface runoff, thereby accelerating erosion rates (Lal, 1991; Montgomery, 2007; Subbulakshmi et al., 2009; Lal, 2020).

Acidification and loss of organic matter worsens soil stability, increases erosion vulnerability, and reduces water retention, affecting plant growth and agricultural productivity (Jie et al., 2002; Bot and Benites, 2005; Šarapatka, and Bednář, 2015; Lal, 2015a; Bednář and Šarapatka, 2018; Chalise et al., 2019; Lal, 2020). Groundwater levels and water retention significantly affect soil-water relationships and degradation processes (Emadodin et al., 2012; Li et al., 2015; Dai et al., 2020). Rising groundwater levels can lead to waterlogging (Hillel et al., 2008; Awad and El Fakharany, 2020) and soil salinization (Emadodin et al., 2012; Singh, 2013; Singh, 2015), reducing crop productivity and increasing soil degradation (Taddese, 2001).

Implementing soil conservation measures, including crop rotation and the incorporation of organic amendments and crop residues is essential for mitigating or reversing soil degradation (Morgan, 2005; Leteinturier et al., 2006; Zuazo and Pleguezuelo, 2009; Lal and Stewart, 2011). These practices minimize erosion, improve soil structure, increase organic matter content, enhance water retention capacity, and promote nutrient cycling (Blanco-Canqui and Lal, 2009a, 2009b; Lal, 2015a). Incorporating organic amendments improves soil porosity and decreases soil bulk density, enhancing hydraulic conductivity (Spaans et al., 1989; Naveed et al., 2014; Dong et al., 2022). Saturated hydraulic conductivity (Ks) and water retention capacity increases with organic amendments due to improved porosity, benefiting plant growth (Aggelides and Londra, 2000; Marinari et al., 2000; Nyamangara et al., 2001; Ferreras et al., 2006). Proper crop rotation can improve long-term soil fertility, aggregate stability, and landscape diversity, thereby preventing soil erosion (Morgan, 2005; Leteinturier et al., 2006; Peltonen-Sainio et al., 2019). There is a need for a reliable assessment of the impact of various crop rotation patterns on soil erosion at a regional level to understand climate change mitigation and hydrological processes (Alewell et al., 2019). Cover crops and crop residues can enhance soil aggregation, increase organic matter content, and improve water infiltration rates, mitigating soil degradation (Blanco-Canqui and Lal, 2009a, 2009b; Mandal et al., 2021). Vegetation cover, including the type and density of plant species, plays an important role in regulating soil moisture and reducing erosion (Zuazo and Pleguezuelo, 2009; Lal and Stewart, 2011). While these measures improve water retention and infiltration rates initially, their longer-term effects, especially concerning different irrigation practices and non-irrigated lands, need further exploration (Schneider et al., 2009; Lim et al., 2016).

Conservation agriculture, with minimal soil disturbance, diversified crops, and permanent cover, reduces erosion rates and enhances soil quality (Lal, 2015a). Precision agriculture, encompassing practices like site-specific nutrient management and variable-rate irrigation, optimizes resource use efficiency and reduces soil degradation risks (Bhattacharyya et al., 2015; Gomiero, 2016). Different land use systems affect soil physical quality, necessitating further investigation to better understand soil functions and processes (Mohawesh et al., 2015; Deng et al., 2016; Hebb et al., 2017; Farahani et al., 2019). Innovative approaches, such as geophysical methods (Hu et al., 2011) and non-destructive measurements (Veldkamp and O'Brien, 2000; Ju et al., 2010) are being explored, aiding in sustainable irrigation management (Hendeley, 2009).

There is a growing emphasis on the modernization and sustainable management of irrigation systems (Schneider et al., 2009; Lim et al., 2016). In addition to conservation agriculture and precision agriculture, researchers are exploring various innovative soil water management practices to address challenges, such as surfactant applications. These surfactants, often based on Alkyl Block Polymer (ABP) or Polyoxyalkylene polymer (PoAP), enhance soil properties, improving re-wettability, infiltration rates, and soil hydration (Cisar et al. 2000; Dekker et al. 2005; Oostindie et al. 2008). Recent studies have highlighted changes in hydrophobicity and organic carbon content (Chu and Chan, 2003; Song et al. 2018), aiming to explore its effects on hydraulic conductivity, nutrient distribution, and organic carbon fractions (Banks et al., 2015; Peng et al., 2017).

Hydrophysical properties of soils are essential for sustainable agriculture and effective water management (Liang et al., 2016; Mandal et al., 2021) and understanding soil hydraulic properties is essential for effective irrigation planning, hydrologic modelling, and preventing further soil degradation (Ventrella et al., 2019; Dong et al., 2022). A major challenge lies in the lack of information on the soil water retention curve (SWRC), making it difficult to assess and predict changes in soil water dynamics that impact agricultural practices (Patil et al., 2011).

Pedotransfer Functions (PTFs) serve a vital role in estimating soil hydraulic properties (Minasny, 2000), including the SWRC and Ks (Salazar et al., 2008; Mihalikova et al., 2013;

Mihalikova et al., 2014). PTFs utilize various soil properties as input predictors, such as soil texture, dry bulk density and organic carbon content, to enhance hydrological modelling accuracy (Wösten et al., 1999; Nemes et al., 2003; Saxton and Rawls, 2006; Weynants et al., 2009; De Lannoy et al., 2014). Furthermore, PTFs have been adapted to consider factors like irrigation and tillage practices, enabling more precise estimations and support for sustainable soil management (Mapa et al., 1986).

Global efforts to combat soil degradation through sustainable land management practices are crucial for long-term food security, environmental sustainability, and the mitigation of degradation risks (Bindraban et al., 2012) particularly in regions marked by intensive agriculture, high population densities, and limited resources for sustainable land management (Oldeman et al., 1991). Various models, such as the Soil Degradation Model of the Czech Republic, assess multiple degradation factors at a local level (Šarapatka et al., 2018). Sustainable land management practices benefit soil health, agricultural productivity, climate change mitigation, and adaptation. Healthy soils act as carbon sinks, reduce greenhouse gas emissions, improve water retention, and enhance ecosystem services (FAO, 2015; Minasny et al., 2017; Lal, 2020). This substantial carbon sink operates in a delicate balance with other environmental pools, making it highly susceptible to changes in land use (Schlesinger, 1995). Any disturbance to the soil system that accelerates mineralization rates within the carbon pool results in reduced carbon content in the soil and the subsequent release of carbon dioxide into the atmosphere (Smith, 2012). For example, agricultural activities, especially those involving tillage, can swiftly deplete levels of soil organic carbon. Lal (2013) provides a comprehensive examination of the significance of the soil organic carbon pool in the context of climate change, shedding light on the potential implications of alterations in land use for greenhouse gas emissions (Montanarella and Alva, 2015).

Soil degradation contributes to a notable reduction in crop yields (estimated between 12.7% to 30%) and incurring substantial economic costs (Oldeman, 1998; Montanarella, 2007) affecting land productivity and leading to socio-economic consequences (Bajocco et al., 2011). Raising awareness about soil degradation among policymakers, farmers, and the public is essential; collaborative efforts are needed to develop supportive policies and integrate soil conservation practices into agriculture (Bindraban et al., 2012; Hurni et al., 2015). Prioritizing soil health and sustainable land management preserves hydrophysical properties, enhances agricultural productivity, and secures the well-being of current and future generations.

Continuous research focused on understanding and addressing degradation processes in irrigated and irrigable soils enables us to understand the complex interactions between soil, water, and agricultural practices. Incorporating advances in modelling, and sustainable strategies allows us to mitigate soil degradation and ensure the sustainable use of soil and water resources for agriculture; adopting conservation agriculture and precision techniques enables us to combat soil degradation, promote sustainable land management, and optimize resource efficiency, soil management and farming systems, play pivotal roles in soil quality deterioration worldwide (Doran and Parkin, 1997). This promotes long-term food security, environmental sustainability, and agricultural system resilience.

1.2. Hydrophysical Properties of Soils

Hydrophysical properties of soils are paramount for comprehending soil water interactions and their profound implications for agricultural systems. These properties encompass a multitude of factors, each with its unique significance in determining how soils function and how they respond to various environmental and management factors. Soil hydraulic properties exhibit spatial variability, as noted by many researchers (Strock et al., 2001; Coutadeur et al., 2002; Horn, 2004; Strudley et al., 2008), and they are significantly impacted by factors such as soil texture, dry bulk density (BD), soil structure, and soil organic matter content (Bagarello and Sgroi, 2007; Petersen et al., 2008).

Soil texture, as classified by the USDA (1951), is often represented by the content of sand, silt, and clay fractions. These fractions define the soil's physical composition, with sand particles measuring between 2.0 and 0.05 mm, silt particles between 0.05 and 0.002 mm, and clay particles smaller than 0.002 mm. This composition of sand, silt, and clay plays a major role in the relationship between soil water potential and soil water content (Saxton et al., 1986). Among the texture factors, clay content stands out as the most influential, this significance of clay content in hydraulic characteristics was underscored by Cosby et al. (1984) through regression and discriminant analysis. Soil texture significantly governs essential soil hydraulic properties including saturated hydraulic conductivity (Ks), unsaturated hydraulic conductivity (K(h)), soil water retention curve (SWRC), and air entry pressure value (Wösten et al., 2001; Li et al., 2014). Moreover, it’s worth noting that the average pore size and distribution exhibit a strong correlation with the particle size distribution, as outlined by Campbell (1985). Understanding the morphology and stability of the soil pore network is paramount and soil structure has equally important effect as the texture.

Soil structure can be defined in two ways: it refers to the shape, size, and spatial arrangement of individual soil particles and clusters of particles (aggregates), or it describes the combination of various pore types with solid particles (aggregates) (Blahovec and Kutílek, 2002). Soil structure and the formation of aggregates are dynamic aspects shaped by soil parent material, climate, and agricultural practices. However, due to the inherent opacity of soil, accurately quantifying the relevant soil structures has proven to be a challenging task (Weber et al., 2023). Notably, clays with shrink/swell properties can profoundly influence the natural variability of soil structure and how soil hydraulic properties respond to various management practices (Horn et al., 1994; McGarry et al., 2000). There is a growing focus on measuring pore space to better understand soil structure. The intricate network of pores between individual particles and aggregates is crucial, serving as a vital medium for water and air storage and movement, indispensable for plant roots, microorganisms, and soil fauna (Blahovec and Kutílek, 2002). Soils that are well-structured, containing higher organic matter and lower bulk density, typically possess enhanced water retention capacity. This is attributed to improved soil structure and the increased availability of pore space for water storage (Nemes et al., 2003).

Progress in quantifying soil structure has been notably constrained, especially when investigating pedon and field scales. (Eck et al., 2013). Soil structure data usually covers aggregate characteristics such as size distributions and stability. However, directly relating these properties to soil pores is complex due to a lack of detailed information on aggregate arrangement and packing within a representative soil volume (Sullivan et al., 2022). Even when available, the data often focuses on shallow depths and small samples (Nimmo and Perkins, 2002), limiting a comprehensive understanding of the soil horizon's morphological structure. Consequently, the interconnectedness of pore networks and the spatial variability of soil hydraulic properties at larger scales are often overlooked (Rabot et al., 2018).

1.2.1. Soil Water Retention Characteristics

Soil water retention characteristics, as described by the Soil Water Retention Curve (SWRC), offer essential insights into soil water availability to plants. The SWRC is the relationship between soil water matric potential (or the energy of attraction between soil water and the solid phase of soil) and volumetric soil water content (θ) (cm^3 cm^{-3}) at equilibrium above the reference (zero) level represented by the free water table at atmospheric pressure (Novák and Hlaváčiková, 2019). The mathematical expression of the soil water retention curve function, denoted as (h_w=f (θ)), serves as a critical input for mathematical models used in studying soil water movement. The SWRC is influenced by various soil properties, including particle size distribution, BD, organic matter content, human activities, and natural processes such as wetting and drying cycles and earthworm activity, which collectively impact soil functionality (Ball, 2013; Pla et al., 2017).

To aid in visualizing the region near saturation, the retention curve is commonly depicted on a semi-logarithmic scale as a pF curve (pF = log |h|) (Kutílek, 1978). The curve is often referred to as a pF curve, wherein equivalent pore radii are plotted on the vertical axis, assuming a parallel capillary tube model (Kutílek and Nielsen, 1994). Figure 1 shows the soil water retention curve using a linear scale for pressure head and a logarithmic scale for h. As pressure heads (h) vary over many orders of magnitude and significant changes in θ occur at relatively small values of h, soil water characteristics can only be effectively plotted on a semi-logarithmic scale (Dirksen, 1999).

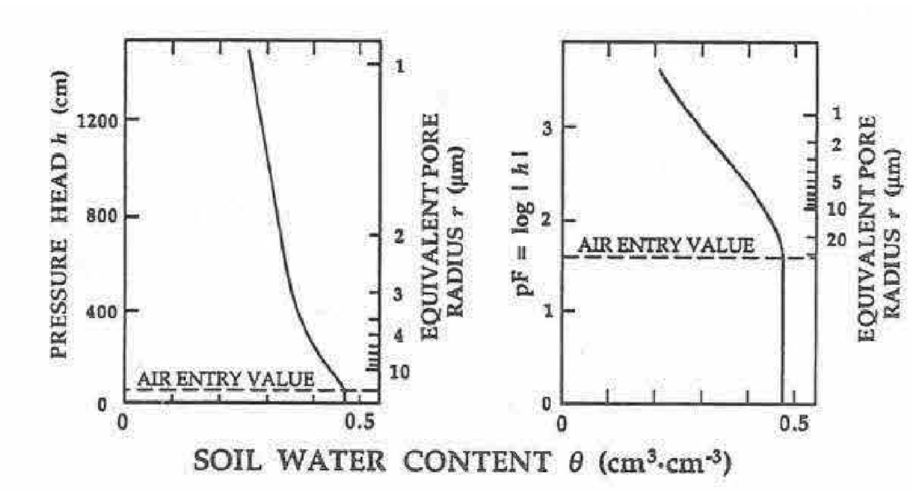

Figure 1. Soil water retention curve using a logarithms scale for h where pF = log |h| (right) and a linear scale for pressure head (h) (cm) (left) (Kutílek and Nielsen, 1994).

Soil water content and matric potentials, commonly referred as "soil water constants," are indicative of water availability to plants (Novák and Hlaváčiková, 2019). These soil water constants represent specific soil moisture levels, obtained through well-defined methodologies, despite not having strict physical definitions. These soil water constants, including Field Capacity (FC), Wilting Point (WP), and Available Water Capacity (AWC), are widely recognized and utilized globally. The Retention Water Capacity (RWC) and Maximum Capillary Water Capacity (MCWC), specific soil water constants for the Czech Republic, offer practical and cost-effective alternatives to the complete soil retention curve measurement.

FC signifies the maximum soil water content (θ_{FC}) soil can hold against the force of gravity after excess water has drained away (Veihmeyer and Hendrickson, 1927; Cassel and Nielsen, 1986), but determining FC in the field is approximate due to dynamic field conditions. FC usually corresponds to a pF value between 2.00 and 2.70, in calculations and estimates, it is important to connect FC with suction pressures. Coarse-textured soils typically achieve FC at -5 to -10 kPa, medium-textured soils at around -33 kPa, and fine-textured soils at -50 kPa (Cassel and Nielsen, 1986). Factors like intense rainfall, soil properties (including hydraulic gradient, hysteresis, soil profile layering, swelling and shrinking, as well as the presence of impermeable layers or high groundwater levels), and topography influence the duration of water saturation, making FC variable.

WP represents the soil water content (θ_{WP}) at which plants experience permanent wilting (Kutílek and Nielsen, 2015), often observed at a matric potential $h_w=10^{4.18}$ cm (pF = 4.18 which corresponds to a suction pressure of -1500 kPa or a pressure head of -15000 cm, -15 bar or a relative vapor pressure of 0.98 on the desorption branch of the adsorption isotherm) as proposed by Briggs and Shantz in 1912. Defining WP precisely is a challenge due to the complex interplay of these multifaceted elements, such as, root depth, plant coverage, and microclimate (Cassel and Nielsen, 1986). Various methods can be employed for approximate calculations of the WP. One approach involves estimating it as one and a half to two and a half times the hygroscopicity value. Another method utilizes equations proposed by Solnař or Váša, which are linear regression relationship between soil water content representing WP and fine particle size fraction, which are soil particles < 0.01 mm (%) (Kutílek, 1978).

AWC is a term used to describe the range of soil water contents (θ_{AWC}) that are accessible to plants within the root layer. This capacity is typically assessed between the field capacity (θ_{FC}) and the wilting point (θ_{WP}), it represents the amount of water in the soil that remains usable by plants over an extended period, and it is calculated as (Eq. 1):

$$AWC = FC - WP \qquad (1)$$

The definitions of FC and WP may vary across different countries; however, the AWC remains a valuable parameter for regional studies concerning soil moisture deficit, irrigation intervals, agro-ecological zoning, assessment of agricultural production potential, and simulation of global landscape changes influenced by economic factors and climate change. In various regions, common intervals utilized to define available water capacity include, for instance, pF

1.70-4.18 in the UK; pF 2.00-4.18 in the Netherlands; and pF 2.52-4.18 in the USA (Batjes, 1996).

RWC, as defined by Kopecký, and MCWC, as defined by Novák, are soil water constants determined in the laboratory using well-defined methodologies. This approach eliminates the need to rely on the challenging process of obtaining FC, which has a long history of use in the Czech Republic as an approximation of FC (Drbal, 1971; Vopravil et al., 2020; Spasić et al., 2023; Almaz et al., 2023b). The RWC of soil, results from the attractive forces between the solid and liquid phases, enabling the soil to retain water despite the effects of gravity, evaporation, and plant root uptake.

The soil water retention curve often exhibits strong hysteresis, leading to significant differences between the drainage and wetting behaviors (Hillel, 1980; Hillel, 2003; Likos and Lu, 2004). Hysteresis results from various factors, including air entrapment in blind pores, variations in pore diameters, and differences in wetting angles during water advancement on dry soil particles compared to water recession from a moist surface (Kutílek, 1978).

The underlying mechanisms responsible for these hysteretic responses have been extensively identified, including potential differences in advancing and receding solid-liquid contact angles, changes in pore structure due to wetting and drying, air entrapment, capillary condensation, and thixotropic or aging effects, which are influenced by the wetting/drying history (Hillel, 1980; Likos and Lu, 2004). These mechanisms are affected by the wetting and drying history, leading to complex relationships between parameters such as θ, θ_w (wetting moisture content), θ_{wr} (residual moisture content), θ_s (saturation moisture content), and θ_{Ar} (representing the air-entrapped volumetric domain between θ_s and θ_w). These relationships are vital for understanding how soil moisture content changes during wetting and drying processes. Hysteresis is associated with primary drainage and primary wetting curves (PDC and PWC, respectively) and main drainage and wetting curves (MDC and MWC, respectively). Scanning wetting and scanning drainage curves (SWC and SDC, respectively) further illustrate these complex behaviours. When a previously dry sample is rewetted, it may not reach the original θ_s but instead reaches a lower level (θ_w), indicating the persistent influence of hysteresis. These intricacies in soil moisture behaviour are essential to consider when studying the dynamics of soil water content during wetting and drying processes (Kutílek and Nielsen, 1994). Figure 2 provides a visual representation of this hysteresis phenomenon (Luckner et al., 1989; Kutílek and Nielsen, 1994), where different curves and parameters help elucidate the relationships between soil moisture contents during wetting and drying.

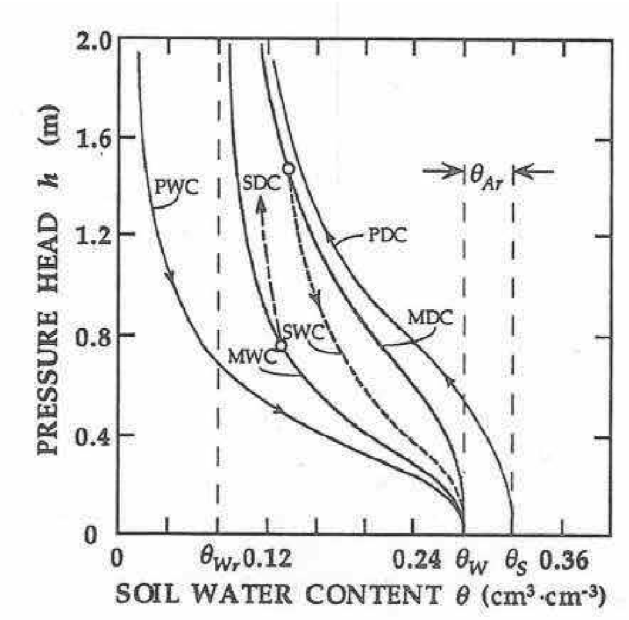

Figure 2. Hysteresis of the SWRC for a coarse-textured soil (Luckner et al., 1989). PDC is the primary drainage curve, PWC the primary wetting curve, MDC the main drainage curve, MWC the main wetting curve, SWC a scanning wetting curve and SDC a scanning drainage curve (Kutílek and Nielsen, 1994).

1.2.1.1. Determination of Soil Water Retention Curve

Laboratory techniques play a crucial role in establishing the soil water retention curve. The measurements differentiate between drainage, wetting, or transitional branches. The method's measurement range is of utmost importance. When determining the retention curve for the entire range of soil moisture usable by plants (i.e., pressure heads from 0 to -15000 cm, sometimes more), a typical approach involves combining two methods, such as the sand/kaolin box, temp cell (Klute, 1986) and pressure plate apparatus (Richards, 1941).

A modern and efficient approach, the evaporation method (Schindler and Müller, 2006), is utilized in commercial devices like HYPROP (Hydraulic Property Analyzer) by METER Group Inc. (Pullman, WA, USA). This method rapidly determines field capacity but involves higher costs and requires careful setup. Recent studies, like Haghverdi et al. (2018), highlight the increasing importance of HYPROP's automated benchtop system for high-resolution water retention data in soil hydraulic property analysis.

1.2.1.2. *Functional Relationships for Describing the Soil Water Retention Curve*

In simulation modelling, an analytical expression of the SWRC is necessary. Among several mathematical functions available, the most used one is the van Genuchten relationship (1980), which can be combined with the Mualem model (1976) for the indirect derivation of unsaturated hydraulic conductivity. According to Cornelis et al. (2005), this relationship (Eq. 2) generally, provides the best fit to experimentally obtained data.

$$\theta = \theta_r + \frac{(\theta_s - \theta_r)}{(1+(\alpha|h|)^n)^{1-1/n}} \qquad (2)$$

where: $|h|$ – absolute value of the actual matric head (cm); θ – actual soil water content ($cm^3\ cm^{-3}$); θ_r – model parameter expressing the residual soil water content ($cm^3\ cm^{-3}$); θ_s – model parameter expressing the saturated soil water content ($cm^3\ cm^{-3}$); α – shape factor (1/cm); n – shape factor (–).

The typical graph of function exhibits an S-shaped curve. The four independent parameters θ_r, θ_s, α, and n are determined by fitting experimentally obtained points of moisture dependence on pressure head $\theta(h)$. Among these four parameters, the saturated moisture content θ_s is usually readily available as it can be easily measured and belongs to standard values determined in hydropedological laboratories.

The parameter θ_r, representing the residual moisture content, is defined as the moisture content at which the gradient ($d\theta/dh$) becomes zero (except in the saturation region where the gradient is also zero). From a practical perspective, the residual moisture content can be identified as the moisture content at high negative pressure head values, such as the wilting point (h = -15000 cm). In some cases, the residual moisture content is not directly measured. Instead, it can be estimated by fitting the measured retention points using the method of least squares with the help of computer programs like RETC (van Genuchten et al., 1991). Table 1 presents van Genuchten parameters for American soil texture classes as defined by USDA (1951). On the left side, it includes parameters used by the RETC parameterization program (van Genuchten et al., 1991) as initial parameter estimates before undergoing optimization. These data originate from the parameterization of 5350 soil horizons in the USA as conducted by Rawls et al. (1982). The right side of the table displays parameters employed by the Rosetta neural network (Schaap et al., 2001), which are derived from the American NRCS database.

Table 1. van Genuchten parameters for USDA soil texture classes (van Genuchten et al., 1991; Schaap et al., 2001).

Texture	RETC				Rosetta			
	Θ_s	Θ_r	α	n	Θ_s	Θ_r	α	n
Sand	0.43	0.045	0.145	2.680	0.375	0.053	0.035	3.180
Loamy sand	0.410	0.057	0.124	2.280	0.39	0.049	0.035	1.747
Sandy loam	0.41	0.065	0.075	1.890	0.387	0.039	0.027	1.448
Loam	0.43	0.078	0.036	1.560	0.399	0.061	0.011	1.474
Silt	0.46	0.034	0.016	1.370	0.489	0.05	0.007	1.677
Silt loam	0.45	0.067	0.02	1.410	0.439	0.065	0.005	1.663
Sandy clay loam	0.39	0.1	0.059	1.480	0.384	0.063	0.021	1.330
Clay loam	0.41	0.095	0.019	1.310	0.442	0.079	0.016	1.415
Silty clay loam	0.43	0.089	0.01	1.230	0.482	0.09	0.008	1.520
Sandy clay	0.38	0.1	0.027	1.230	0.385	0.117	0.033	1.207
Silty clay	0.36	0.07	0.005	1.090	0.481	0.111	0.016	1.321
Clay	0.38	0.068	0.008	1.090	0.459	0.098	0.015	1.253

The parameter α describes soil's largest connected pores. Higher α values mean less capillary rise above the water table. The fourth parameter n portrays pore size distribution. Higher n values indicate a narrow range found in coarse-grained soils, while lower n values imply a broader distribution, typical in fine-grained soils (API, 2006). Figure 3 visually illustrates how these parameters affect the equation (Eq. 2).

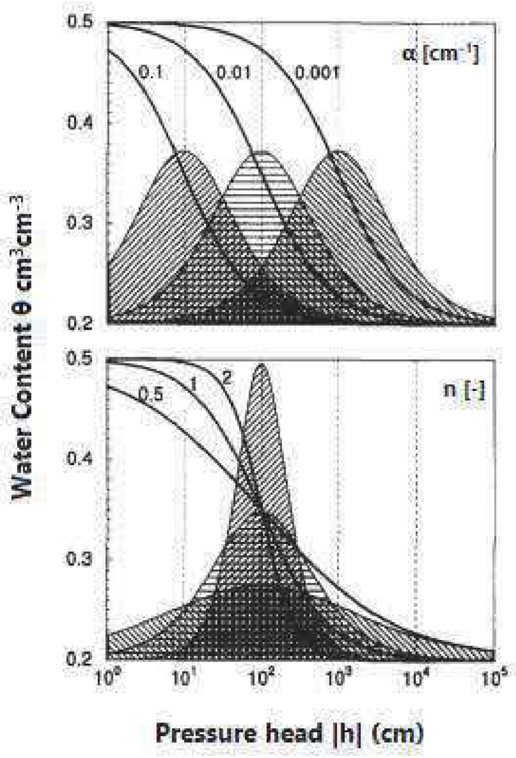

Figure 3. Influence of the parameters α and n on the shape of equation (Eq. 2) and their first derivatives representing pore size distribution (Scheinost et al., 1997).

1.2.2. Soil Hydraulic Conductivity

Hydraulic conductivity, denoted as K and measured in international system of units (SI units) of meters per second, is a property of porous materials, soils, and rocks. It defines the material's ability to allow the passage of fluids, typically water, through the pore space (Saravanan et al., 2019). Soil hydraulic conductivity is a significant soil property that regulates the transport of water and solutes within soils (Poulsen et al., 1999).

In soil physics, unsaturated soils, which have only partially filled pore volume with water, exhibit lower hydraulic conductivity than saturated soils. This is because only water-filled pores contribute to water flow (Koorevaar et al., 1983). The presence of both air-filled pores and capillary forces in unsaturated soil significantly influences water retention and hydraulic conductivity, making it more challenging to characterize water movement compared to saturated soil. Understanding unsaturated hydraulic conductivity (K(h)) is vital, as most plants thrive in unsaturated soil, relying on air for respiration and growth (Novák and Hlaváčiková, 2019).

Ks characterizes the ease with which water moves through the pores of saturated soil or rock (United States Department of Agriculture, 2022). Particularly crucial during precipitation, snowmelt, flooding, and irrigation events, Ks significantly influences water flow behavior, infiltration rate, runoff generation, and deep drainage, making it a pivotal soil property (Gamie and De Smedt 2018; Araya and Ghezzehei, 2019), and is influenced by various factors, including soil texture, structure, and organic matter content (Jury and Horton, 2004). Various techniques estimate Ks, including infiltration tests, laboratory measurements (Klute 1986), and predictive models; however, it is important to note the non-existence of any standardized reference method for Ks determination (Batkova et al., 2022). Nevertheless, these methods provide insights into Ks and aid in decision-making for water management. Incorporating temporal dynamics of soil hydraulic properties improves soil moisture predictions, enhancing water management strategies and supporting sustainable agriculture (Schwen et al., 2011; Alletto et al., 2015; Sipek and Tesar, 2017).

Ks stands as a fundamental and extensively utilized soil parameter, finding widespread applications across various geotechnical, environmental, and water investigations and models (Schaap et al., 2001; Araya and Ghezzehei, 2019; Tuffour et al., 2019). However, due to its inherent high spatial and temporal variability, hydraulic conductivity tends to be an inadequate indicator of soil hydraulic response to management practices. This is because the natural variability often masks the effects of specific treatments, making it challenging to discern treatment-induced changes (Strudley et al., 2008).

1.2.3. Influence of Soil Organic Matter on Soil Hydraulic Properties

Soil organic matter (SOM) significantly impacts soil hydraulic properties, improving water-holding capacity and hydraulic conductivity (Hillel, 2003). SOM, along with clay minerals, modifies pore space changes with changing soil moisture (Fuentes et al., 2009), by augmenting water and nutrient retention, a cornerstone for robust plant growth (Power and Prasad, 1997). It enhances nutrient retention by increasing cation exchange capacity (CEC), vital for sustaining plant health (Hillel, 2003).

Examining potassium permanganate oxidizable organic carbon (POXC) variations serves as an indicator of the labile carbon pool, encompassing a mixture of water-repellent and water-attracting compounds formed during the initial decomposition of SOM. (Bongiorno et al., 2019). Water-soluble organic carbon (Cws) is a part of Total Organic Carbon (TOC) that dissolves in water at room temperature. It includes substances like sugars, amino acids, and other organic compounds, which microbes can easily access, aiding soil fertility and nutrient cycling. Conversely, hot water-soluble organic carbon (Chws) contains a greater variety of complex organic compounds (Uchida et al., 2012). These complex organic compounds include microbial biomass carbon, root exudates, amino acids, and carbon linked to soil enzymes (since many enzymes are denatured at high temperatures), which allows Chws analysis to cover significantly more carbon than Cws analysis can.

Elevated POXC levels may reduce saturated hydraulic conductivity (Ks) due to bioclogging, as previous studies have indicated (Hallett et al., 1999). Soil bacteria form biofilms that cover pore walls with exopolymer glycocalyx, reducing water flow space (Peng et al., 2017). This biofilm formation may also change soil swelling properties and the dispersion of colloidal particles, possibly impacting Ks. The observed decline in Ks values from the study by Almaz et al., (2023a) aligns with results from the unsaturated hydraulic conductivity (K(h)) tests conducted in laboratory settings using non-hydrophobic loamy sand soils, both treated soils (with the non-ionic surfactant H2Flo, ICL-SF Inc.) and untreated soils. Similar outcomes have been highlighted in various studies over the past two decades, particularly in non-hydrophobic soils (Mobbs et al., 2012; Bashir et al., 2020). Bashir et al. (2020) linked reduced hydraulic conductivity to slower vertical water and surfactant movement and increased lateral dispersion. While direct comparative scenarios between Ks and organic carbon fractions (OCFs) are scarce in the literature, Almaz et al. (2023a) suggested moderate to strong, yet divergent correlative links between OCFs and Ks.

1.2.4. Agricultural Practices and Tillage

Tillage stands as the most extensively studied management practice influencing soil hydraulic properties (Strudley et al., 2008). Gupta et al. (1991) provided an insightful review of models for predicting the impact of tillage on various soil properties, including dry BD, hydraulic and thermal conductivity, and water retention characteristics. Despite the passage of over decades, a significant portion of the methods outlined by Gupta et al. (1991) still necessitates rigorous laboratory and field-testing, underscoring their ongoing importance in the advancement of the field.

Practical operations like repeated tillage (Blahovec and Kutílek, 2002), re-compaction, and harvest can have negative effects on soil physical properties. These actions, including shifts in aggregate stability, decreased SOM, changes in soil fauna activity, and effects on root growth and decay, often lead to unfavourable soil porosity conditions for crop growth (Pagliai et al., 1983; 1984; 1989; Shipitaio and Protz, 1987). This becomes more pronounced with alterations in land utilization and tillage procedures, as they can significantly impact soil hydraulic characteristics (Meurer et al., 2020a; Meurer et al., 2020b; Vereecken et al., 2010). Moreover, these intermittent processes, occurring throughout the year or across different seasons, can profoundly affect soil hydraulic properties (Messing and Jarvis, 1993; Horn et al., 1994; Bodner et al., 2013; Sandin et al., 2017).

1.3. Pedotransfer Functions for Estimating Soil Properties

1.3.1. Definition and Purpose of PTFs

Estimating soil properties from more easily measurable soil properties has been a historical challenge in soil science. Early in the twentieth century, Briggs and Lane (1907) and Veihmeyer and Hendrickson (1927), pioneered relating soil moisture characteristics to soil texture using regression. These equations became fundamental in soil classification and mapping efforts.

Initially proposed by Bouma (1989), pedotransfer functions (PTFs) are empirical or statistical models that bridge the gap between the scarcity of direct soil property measurements by translating available soil data into the necessary information for assessing soil properties (Minasny et al., 1999). With the advancement of computing technology, PTFs have evolved, making it more feasible to use soil hydraulic properties to simulate the soil environment (Minasny, 2000). These functions have become indispensable tools in soil science research, with a particular focus on applications such as hydrological modeling, land management, and environmental applications (Parsuraman et al., 2007; Vereecken et al., 2010; Van Looy et al., 2017).

To ensure accurate estimations, the applicability of PTFs should ideally be assessed in contexts similar to those where they were developed to avoid extrapolation errors (Wösten et al., 1998; Nemes et al., 2003). Pachepsky and Rawls (1999; 2004) stressed in their review on PTFs that these functions are most effective when applied to regions or soil types like the ones in which they were originally developed. This approach helps avoid potential biases and ensures the reliability of PTFs (McBratney et al., 2002; Nemes et al., 2003). Calibration and validation using field data from the target region are essential steps in evaluating the accuracy and applicability of the PTFs (Bouma, 1989; Wösten et al., 1999; Patil and Chaturvedi, 2012). Adding to this perspective, Gerke et al. (2022) highlighted a critical factor - the potential limitations of machine learning (ML) models when trained on data from a specific geographical region.

1.3.2. Classifying and Using Pedotransfer Functions in Soil Properties Estimation

Comprehending and effectively utilizing PTFs involves classifying them based on various criteria, offering insights into their nature and applicability. Two fundamental classifications are commonly employed: (i) based on the nature of predictors and (ii) based on the nature of the estimated data.

Bouma (1989) categorized PTFs based on the nature of predictors into two main types: (a) class-PTFs, establish relationships between modelling parameters and classes of soil properties outlined in soil surveys (Bouma, 1989); and (b) continuous PTFs, which utilize variables such as clay, sand, or organic matter content as continuous inputs in multivariate regression or machine learning models to estimate water retention curve model parameters or soil water at specific matric potentials (Rubio et al., 2008). Class-PTFs are particularly suitable for predicting soil hydraulic characteristics at national and continental scales due to the typically less detailed data available at these scales (Wösten et al., 1995; Al Majou et al., 2008). Continuous PTFs have evolved to cover a broader range of soil properties and functions (Breeuwsma et al., 1986; McBratney et al., 2002), making them increasingly versatile.

Within the classification based on the nature of the estimated data, continuous PTFs can be further categorized into (a) point-based and (b) parametric PTFs (Tomasella et al., 2003; Vereecken et al., 2010). Point-based PTFs are empirical equations that estimate soil moisture at predefined potentials, while parametric PTFs estimate parameters of a certain functional model, often the van Genuchten equation (Eq. 2), offering valuable insights into soil property estimation, facilitating large-scale assessments and decision-making processes. Parametric PTFs are advantageous for analyzing transport processes, offering continuous hydraulic property functions. They allow the integration of moisture measurements at different potentials during derivation, eliminating the need for specific potential measurements (Minasny et al., 1999; Tomasella et al., 2003).

By utilizing pedotransfer functions, soil properties can be estimated quickly and cost-effectively, making them valuable tools for large-scale assessments and decision-making processes. However, it is essential to consider the limitations and applicability of each classification of PTFs to ensure their appropriate use in soil property estimation.

1.3.3. Optimizing Soil Property Estimation: Advanced Data Grouping and PTFs

Prior to deriving PTFs, the database of measured soil hydraulic properties can be grouped into soils that are more similar. This approach offers the advantage of providing more stable and consistent correlations of hydraulic properties with other soil properties within soil groups that have similar flow processes. As a result, more accurate PTFs can be derived for individual groups rather than for the entire database (Bruand, 2004a).

Studies by Franzmeier (1991) and Wösten et al. (1990) have shown that grouping soils based on genetic soil horizons and parent rock is more appropriate than grouping by texture classes. Additionally, Wösten et al. (1990) experimented with grouping soils based on the functional behaviour of different horizons, where similar simulated flow behaviour led to the grouping of different soil horizons.

There are three main approaches considered for data grouping (Wösten et al., 2001):

1. Grouping data and calculating the average hydraulic properties for each defined group: In this approach, no further pedotransfer functions are derived within the groups. The name or number of the group is used as a nominal illustrative variable, and the texture class based PTFs belong to this category.

2. Grouping data and deriving PTFs separately for each defined group using different soil properties according to the groups.

3. Deriving pedotransfer equations for the entire data set without dividing it into groups.

For instance, Schillaci et al. (2021) emphasized the significance of data grouping in their study on predicting BD in Mediterranean agro-ecosystems. Notably, their Artificial Neural Network (ANN) PTF showcased superior performance compared to other approaches, highlighting the effectiveness of data grouping strategies for accurate property estimation. In a similar vein, Zhang et al. (2020) advocated for data grouping through their Hierarchical Ensemble Model, utilizing 13 PTFs to estimate global soil water retention. By leveraging ensemble modelling and grouping, they achieved more precise estimates of soil water retention, reducing uncertainty in predictive models. Furthermore, Ghanbarian and Yokeley (2021) proposed a novel approach for soil classification based on hydraulic conductivity data, underlining the practical applications and benefits of effective data grouping. Their classification methodology, relying on critical path analysis and hydraulic conductivity curves, showcased how similar critical pore sizes at the same effective water saturation could lead to a cohesive soil classification.

1.3.4. Advancements in PTFs for Estimating Soil Hydraulic Properties

Researchers have primarily focused on developing PTFs for estimating soil hydraulic properties in various geographical areas and soil types, aiming to identify the most relevant and influential soil properties as input predictors (Nemes et al., 2002). Subsequent advancements led to more sophisticated approaches, such as describing the soil water retention curve (Brooks and Corey, 1964; van Genuchten, 1980), which greatly improved the accuracy of hydrological modelling and environmental assessment.

Addressing the unavailability of predictor data, researchers have modified PTFs to incorporate a hierarchical methodology (Schaap et al., 2001; Patil et al., 2010; Botula et al., 2012) and Schaap et al. (1998) developed a system of hierarchical PTF rules (PTR) to predict available water for main soil series worldwide. This hierarchical approach enables PTFs to adapt to varying input data availability by starting with minimal required information, this method is highly significant, following the principle that "if measuring the predictor is simpler than measuring what's being predicted, there's no need for a prediction" (McBratney et al., 2002; Minasny and Hartemink, 2011).

A wide range of soil properties have been utilized as input predictors in PTFs. These include soil texture-based approaches and the percentages of sand, silt, and clay (Bloemen, 1980; Cosby et al., 1984; Rawls and Brakensiek, 1985; Saxton et al., 1986; Campbell and Shiozawa, 1992; Nemes et al., 2003; Palladino et al., 2022). Additionally, dry BD, organic carbon, and organic matter content have been commonly incorporated as predictor variables (Rawls et al., 1983; Vereecken et al., 1989; Wösten et al., 1999; Saxton and Rawls, 2006; Weynants et al., 2009; De Lannoy et al., 2014). To further improve water retention curve estimations, PTFs have considered morphological properties, clay mineralogy, soil structure, moisture retention points and saturated hydraulic conductivity (Ks) are utilized as additional predictors, capturing fundamental aspects of soil water dynamics (Williams et al., 1992; Paydar and Cresswell, 1996; Schaap et al., 2001; Rawls and Pachepsky, 2002b; Pachepsky and Rawls, 2004; Pachepsky et al., 2006; Nguyen et al., 2015a; Zhang and Schaap, 2017 Vereecken et al., 2010; Jana and Mohanty, 2011; Patil and Singh, 2016; Lehmann et al. 2021). Chemical properties such as calcium carbonate ($CaCO_3$) content and CEC have also been employed as predictor variables in PTFs (Rajkai and Varallyay, 1992; Gomes et al., 2019), the content of $CaCO_3$ has been identified as a relevant predictor in certain PTFs, as it can significantly impact water retention characteristics (Bruand, 2004b; Štekauerová et al., 2002).

For a long time, soil structure has been identified as a critical yet overlooked factor affecting soil hydraulic properties in PTFs (Terribile et al., 2011; Pachepsky and Rawls, 2003). Existing PTFs often inadequately represent soil structure, as highlighted by Vereecken et al. (2019). The inadequate performance of PTFs in predicting saturated and near-saturated hydraulic conductivity can be attributed to the absence of predictors that effectively quantify pertinent soil structures (Vereecken et al., 2010; Jorda et al., 2015; Gupta et al., 2021b). Addressing this deficiency, leveraging data on soil aggregates obtained from field surveys emerged as an appealing solution (Pachepsky and Rawls, 2003).

Particle size distribution (PSD) is one of the fundamental soil properties used as a predictor in PTFs. The physically empirical model introduced by Arya and Paris (1981) leverages the similarity between particle size and SWRC by converting PSD to pore size distribution. This approach proves to be particularly effective in estimating hydraulic properties in sandy and structureless soil materials (Gee and Bauder, 1986; Matula, 1992). Recent studies have further underscored the importance of PSD in predicting soil properties highlighting the critical role of PSD (Abdelbaki, 2018; Amanabadi et al. 2019)

Another important soil property used as a predictor is dry BD, which provides insights into soil compaction and pore space, influencing soil water retention and movement, given the increasing focus on evaluating ecosystem services, soil bulk density holds significant importance as a fundamental attribute for soil functions (Rabot et al., 2018). Notably, environmental processes and agricultural practices introduce significant spatial and temporal variations in soil bulk density, presenting a unique challenge in precisely characterizing this variability (Makovníková et al., 2017). Although dry BD is a crucial parameter, researchers frequently avoid its measurement, especially in large-scale projects where a substantial number of samples are needed (Kaur et al., 2002; Baritz et al., 2010; Nanko et al., 2014; Sevastas et al., 2018). Recent studies further affirm the significance of dry BD as a predictor (Makovníková et al., 2017; Nasta et al., 2020).

Enhancing PTFs to improve hydrophysical estimations involves considering various factors, including irrigation and tillage practices. These additional considerations lead to more precise estimations and support sustainable soil management practices. Irrigation practices significantly modify soil hydraulic properties (Mapa et al., 1986), impacting water movement and availability (Kumar et al., 2022). Kumar et al. (2022) underscored the crucial role of site-specific soil hydraulic properties in determining irrigation thresholds and optimizing practices. They optimized soil hydraulic properties based on topography, soil texture, and historical crop yield, emphasizing the need for zone-specific soil hydraulic properties to tailor efficient irrigation strategies, showcasing improved irrigation practices based on different soil depths and scenarios. Mapa et al. (1986) demonstrated how soil deformation due to wetting and drying cycles alters key hydraulic properties like conductivity and sorptivity, especially post-tillage. Conducted on soils, including Typic Torrox and Vertic Haplustoll, the study highlighted that hydraulic conductivity near saturation is highly sensitive to these temporal changes, decreasing significantly. Including relevant data on irrigation regimes and strategies in PTFs can significantly enhance estimations, particularly for irrigated agricultural lands, enabling a more accurate estimation of soil water retention and hydraulic conductivity in areas where irrigation is a prominent practice (Zhao et al., 2016).

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, the estimation of unsaturated hydraulic conductivity has received less attention in PTFs due to a shortage of relevant data and difficulties in comparing results obtained with different techniques (Minasny, 2000; Nemes et al., 2001).

Saturated hydraulic conductivity stands as a crucial soil property governing water infiltration, surface runoff, pesticide leaching from agricultural areas, and the movement of pollutants from contaminated sites to groundwater (Bagarello and Sgroi, 2007). 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. For instance, Gupta et al. (2021a) demonstrated that relying solely on clay fraction as a predictor for soil hydraulic properties can result in an underestimation of Ks, potentially impacting water distribution across the land surface (Lehmann et al., 2021). Gupta et al. (2022) further emphasized the need for considering mineralogy alongside clay fraction, particularly in tropical regions, to enhance the accuracy of Ks predictions. Their methodology incorporated soil samples from diverse climates, spanning temperate to tropical regions, enhancing predictive accuracy across various biomes. However, a notable challenge remains the spatial distribution and coverage of available soil samples for model training are constrained, emphasizing the need for ongoing efforts in comprehensive data collection, particularly from underrepresented regions.

1.3.5. Methods to Derive Modern PTFs

Developing accurate pedotransfer functions (PTFs) has seen a significant transformation over the years. Initially, PTFs were established through traditional regression techniques, where relationships between soil properties and predictors were expressed by equations (Bouma, 1989; Wösten et al., 1999; Patil, 2012).

In the current focus, modern PTFs have evolved to incorporate advanced machine learning algorithms (Figure 4), offering improved accuracy and flexibility. These algorithms enable us to capture complex relationships between soil properties and predictors without the need for predefined models. Notably, the term "PTFs" is now used more broadly to encompass these newer approaches, even though they may not rely on traditional equations. This distinction underscores the shift from old classifications to a more diverse and adaptable set of methods.

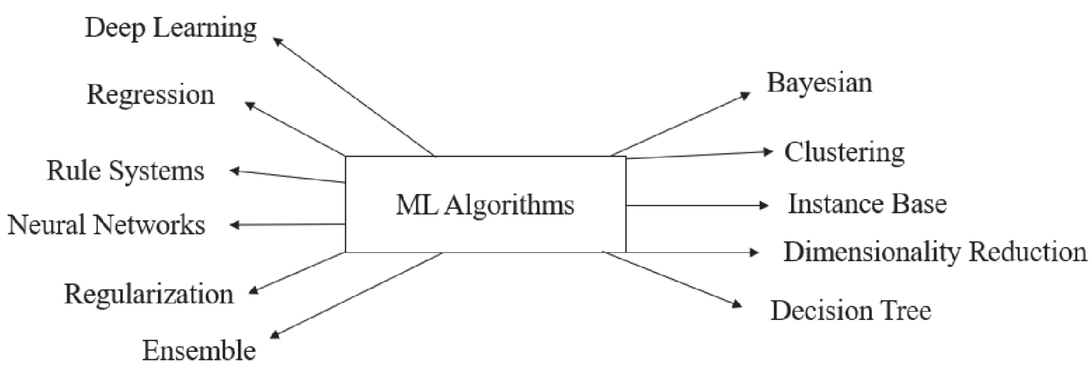

Figure 4. Example of the machine learning algorithms mind map (inspired by Kiadi and Tan, 2018)

Among the various machine learning algorithms, the following are commonly utilized in the development of modern PTFs:

1.3.5.1. Regression Techniques

Regression techniques are widely employed for establishing relationships between predictors and estimands due to their simplicity. Depending on the expected relationship among variables, linear regressions or nonlinear regressions can be utilized. In recent years, several studies have explored the use of regression methods to develop PTFs for specific soil properties (Kotlar et al., 2020). Multiple linear regression is commonly applied for point-based PTFs, while nonlinear regression is more suitable for estimating parametric PTFs (Rawls et al., 1982; Wösten et al., 1999; Minasny, 2000; Šútor and Štekauerová, 2000).

1.3.5.2. Artificial Neural Networks

Artificial Neural Networks are versatile computational models known for their ability to effectively capture intricate input-output relationships (Pachepsky et al., 1996; Schaap and Leij, 1998; Minasny et al., 1999; Minasny and McBratney, 2002; Merdun et al., 2006). They operate without predetermined model concepts and iteratively adjust parameters during calibration to achieve accurate predictions (Haykin, 1994; Maren et al., 2014). ANNs are particularly adept at handling complex relationships and have consistently demonstrated superior performance in estimating soil properties compared to traditional regression-based PTFs (Schaap et al., 1998; Bhattacharya et al., 2021).

1.3.5.3. k-Nearest Neighbor

The k-Nearest Neighbor method is a nonparametric approach, well-suited for estimating soil properties when the underlying relationships are less understood (Nemes et al., 2006; Nemes et al., 2008). By identifying similar objects in memory and deriving estimates based on their likeness, k-NN does not rely on a priori model assumptions, making it valuable when little prior information is available. Researchers have utilized k-NN in various applications, including estimating soil properties and deriving PTFs (Jagtap et al., 2004; Botula et al., 2013; Nguyen et al., 2015b). It has been used successfully in predicting FC and WP with efficiency comparable to advanced neural computing techniques (Nemes et al., 2006; Mihalikova et al., 2014; Miháliková et al., 2016; Duffková et al., 2020). Moreover, k-NN offers simplicity in use and the possibility of appending development datasets, making it an attractive alternative for PTF development (Patil et al., 2011; Patil and Chaturvedi, 2012).

1.3.5.4. Decision/Regression Trees

Decision and Regression Trees offer the ability to partition datasets into homogeneous subsets, allowing for the development of independent PTFs tailored to each subset.

Decision/regression trees allow the partitioning of datasets into homogeneous subsets, enabling the development of independent PTFs for each subset, which is especially useful when distinct dependencies exist within the data (Schaap, 2004). Recursive data partitioning algorithms, such as decision trees, are employed for this purpose, dividing the data into subsets to maximize homogeneity at each partitioning level (Breiman et al., 1984). Each partitioning can be viewed as a branching of a tree (Wösten et al., 2001). These trees can be applied in the context of point-based and parametric PTFs. Strobl et al. (2009) provide a comprehensive review of the key features of recursive partitioning methods. While decision trees are commonly used for continuous response variables, classification trees are more suitable for categorical-dependent variables, minimizing the residual sum of squares to create subsets (Schaap et al., 2004; Strobl et al., 2009). Furthermore, recent progress includes using an ensemble of many regression trees in a procedure called boosting, which was used to identify qualitative/categorical soil properties that help improve the estimation of Ks (Lilly et al., 2008) and derive a PTF of BD for Ks (Jorda et al., 2015).

1.3.5.5. Random Forest

Random Forest, an ensemble of trees, extends the capabilities of a single regression tree (Breiman, 2001) by using multiple trees that consider random combinations of input variables. The resulting model is more robust; however, the method should be used with caution, especially when dealing with noisy data (Segal, 2004) or complex relationships among soil properties and predictors. As a result, Random Forest has gained popularity in recent years and has been successfully applied in various studies (Koestel and Jorda, 2014; Tóth et al., 2014; Szabó et al., 2019; Rastgou et al., 2020).

These machine learning algorithms represent a shift towards more flexible and adaptable PTFs, offering a new perspective on relating soil properties and predictors. They have gained popularity for their ability to improve the precision and dependability of soil property estimations. By incorporating these advanced techniques into the development of modern PTFs, researchers are better equipped to address the complexities of soil behaviour and enhance our understanding of this critical field.

1.3.6. Functional Evaluation of Pedotransfer functions

PTFs are essential in soil science for estimating soil properties, yet they come with inherent limitations and uncertainties. These uncertainties arise from various sources, such as measurement errors in input data, biases in model structure and coefficients (Minasny and McBratney, 2002), the appropriate selection of datasets and the comprehensiveness of input variables (Boschi et al., 2014; 2015). It is essential to provide the uncertainty of the PTFs alongside calibration data summary statistics (McBratney et al., 2002; 2011), enabling model users to account for uncertainties in their analyses. A good model (PTF) should be accurate and reliable: the term accuracy is related to the comparison between predicted and measured values of the soil property of interest, and reliability is related to the evaluation of PTFs on measured values that are different from those that were used to develop the PTFs (Wösten et al., 2001; Patil et al., 2010).

The choice of development method significantly influences PTF accuracy. For instance, when estimating the van Genuchten parameters, Minasny et al. (1999) showed that multiple-linear regression resulted in lower accuracy. Furthermore, the PTF output (e.g., van Genuchten parameters), rather than the input, may be averaged. However, some soil hydraulic properties do not behave linearly over different scales, especially the (unsaturated) hydraulic conductivity or the van Genuchten shape parameters α and n, resulting in considerable uncertainties in water flow predictions (Zhu and Mohanty, 2002; Montzka et al., 2017). Proper consideration of these factors, along with comprehensive evaluation and validation, is crucial for developing robust PTFs that yield reliable soil property predictions.

Exercising caution is necessary when applying PTFs to new data, especially when extrapolating PTFs calibrated with data from different regions or databases. Reliable predictions require limiting extrapolation to similar predictor variable ranges or pedological domains with comparable variations in soil hydraulic properties (Nemes et al., 2003). Regarding this matter, Donatelli et al. (2004) and Schaap (2004) conducted comprehensive reviews of diverse methodologies used to evaluate and quantify the performance of PTFs in predicting soil water retention parameters and hydraulic conductivities.

Contreras and Bonilla (2018) comprehensively evaluated 13 PTFs for predicting soil water content at -33 and -1500 kPa (FC and WP) derived from tropical soils and U.S. soil samples. They used independent Chilean soil data for the evaluation and assessed PTF performance improvement after calibration. Results demonstrated the significant influence of soil types on PTF performance, with notable improvements after calibration. Specifically, Rawls et al. (2004) predicted water content before calibration, with an RMSE of 0.08 for -33 and -1500 kPa, Gupta and Larson (1979) showed the best performance after calibration (RMSE of 0.06 and 0.05, and r^2 values of 0.69 and 0.66 at -33 and -1500 kPa, respectively).

Various statistical indices, such as root-mean-square errors (RMSEs), mean errors (MEs), index of agreement (d), mean absolute error (MAE), correlation coefficient (r), and coefficient of determination (r^2), are used to evaluate, and validate PTFs (Donatelli et al., 2004; Schaap, 2004; Almaz et al., 2023b).

RMSE provides insights into the model's predictive ability, and acceptable values may vary based on the number of data points used in model development and testing (Tomasella et al., 2003; Vereecken et al., 2010; Jana and Mohanty, 2011; Patil et al., 2011, 2012). RMSE is a favoured indicator in evaluating PTFs, as it provides insights into the model's ability to predict away from the mean, emphasizing high values due to the squared differences between observed and predicted values.

The ME compares the mean difference between predicted and observed data, revealing tendencies for overestimation (positive values) or underestimation (negative values) (Benites et al., 2007; De Vos et al., 2005; Nanko et al., 2014), while MAE evaluates bias in prediction by passing the opposite signs of errors (Shein and Arkhangel'skaya, 2006; Sevastas et al., 2018). It is essential to emphasize that the ME represents an average estimation across (N) data points. Consequently, for best performing models, the value of ME should be close to zero (Abdelbaki, 2018); in contrast, the correlation between the observed and predicted data, denoted by the r and r^2 coefficients, is greater when the coefficients signify a stronger correlation (Batkova et al., 2022; Báťková et al., 2023). This discrepancy highlights the need for a comprehensive evaluation and contextual understanding of PTFs to ensure accurate estimations.

Overall, PTFs accuracy varies depending on the development method used, necessitating appropriate model selection to enhance precision and reliability. Thorough evaluation and validation, along with advancements in modelling techniques and data incorporation, contribute to robust PTFs for reliable soil property predictions.

1.3.7. PTFs Look-up Tables, Models and Databases

PTFs can take various forms, such as mathematical formulas, look-up tables, databases, or software integrations. Users often adapt PTFs to meet specific needs, estimating soil properties beyond the initial calibration.

Look-up tables, like those by Baker (1978) and Bouma (1989), are simple and widely used, offering textural class-average hydraulic parameters (Cosby et al., 1984), the Rosetta model H1 (Schaap et al., 2001) is incorporated into variably saturated media simulation models like HYDRUS 1-D, 2-D, and 3-D. Cosby et al.'s (1984) look-up table has applications in land surface modelling, such as the Biosphere-Atmosphere Transfer Scheme by Dickinson et al. (1986; 1993) and the Global Land Data Assimilation System by Rodell et al. (2004) to estimate soil hydraulic parameters.

Environmental and ecosystem management simulation models like DRAINMOD, HYDRUS, EPIC, SPAW, and WEPP utilize PTFs to calculate soil hydraulic properties (Malota et al., 2022; Silva et al., 2020; Turco et al., 2017; Turek et al., 2020). Databases, exemplified by HYPRESCZ (Mihalikova et al., 2013), significantly enhance property estimation precision, improving the reliability of environmental and ecosystem management models. NearriCZ (Duffková et al., 2020; Miháliková et al., 2020) aids in irrigation and crop yield management by providing estimations of critical agronomic hydrological thresholds, encompassing FC and WP.

PTFs look-up tables, databases, and incorporated models, offer valuable insights into soil behaviour for decision-making in soil science and environmental studies. However, their limitations and variability must be considered for reliable application in different contexts.

1.4. Assessing PTF Transferability and Integration in Environmental Models

PTFs have been a cornerstone in soil science, serving not just as an end but as indispensable tools for predicting important soil properties such as available water capacity and hydrophysical properties (Walczak et al., 2004). While accuracy is undoubtedly important in PTFs, their functionality and relevance in practical applications are of equal significance.

These models, while emphasizing accuracy, also find utility in diverse practical applications, particularly within global environmental and ecosystem management models. Discrepancies between PTF-calculated and measured properties often minimally impact model outcomes, underlining the importance of a functional evaluation approach (Vereecken et al., 1992).

The integration of PTFs into environmental and ecosystem management models has enhanced our understanding of water availability, land management practices, and ecosystem services (Vereecken et al., 2010; Jana and Mohanty, 2011). It has shed light on soil-related factors and their roles in ecosystem functioning. For instance, PTFs have been used to estimate soil properties, such as water retention and hydraulic conductivity, allowing researchers to discern the impact of soil conditions on nutrient cycling, plant growth, and ecosystem health (Štekauerová and Šútor, 2004). These insights contribute significantly to decision-making processes concerning sustainable land management, water resource management, and ecosystem conservation. Recognizing the critical role of accuracy and reliability in PTFs, an evaluation framework proposed by Wösten et al. (2001) employs PTFs as input for Earth system models, ensuring a holistic assessment of the entire system's performance. This framework considers accuracy, reliability, and applicability (Vereecken et al., 1992; Xevi et al., 1997).

The adaptability of PTFs across regions and soils has also received attention. Tomasella and Hodnett (2004) addressed unique characteristics of tropical soils using extensive datasets (771 horizons from 249 soil profiles across 22 countries). They developed a novel approach for predicting individual water retention points, demonstrating that tropical soils with low bulk density should be considered separately in PTFs. There is evidence to suggest the potential use of PTFs outside their original geographical development locations, provided soil type and climate comparability (Wösten et al., 2013). Wösten et al. (2013) explicitly investigated the application of PTFs developed for South American soil types to predict measured data in the Limpopo catchment of South Africa. Similarly, Fuentes-Guevara et al. (2022) explored the suitability of translocated PTFs, analyzing input-input and input-output correlations in databases from the development of four PTFs and comparing them with data from their application catchment. They concluded that data correlation similarities, rather than factors like climate, source area, database size, or spatial extent, best explained PTF performance. Further research is needed to validate this transfer learning approach used in soil mapping (Malone et al., 2016) or rely on meta-models (Grunwald et al., 2016). This might allow us to understand under which system conditions PTFs are expected to be similar beyond the limit of local specificity.

PTFs are central to advancing soil science and environmental management, especially when direct measurements are challenging at larger scales. Ensuring their precision, dependability, and suitability necessitates a thorough functional evaluation. Moreover, the development and adaptation of PTFs should account for regional variations to support robust predictions and informed decision-making in diverse contexts. Calibration and validation using field data from the target region remain essential steps to ensure the accuracy and applicability of PTFs.

1.5. Soil Hydraulic Properties Estimates in the Czech Republic

Over the years, substantial progress has been made in the development and application of PTFs to estimate soil hydraulic properties in the Czech Republic (Matula and Špongrová, 2007; Matula et al., 2007; Sněhota et al., 2009; Mihalikova et al., 2013; Mihalikova et al., 2014; Kameníčková and Larišová, 2014; Vlček and Hybler, 2015; Batkova et al., 2022; Báťková et al., 2023).

Matula and Špongrová (2007) found that the continuous PTFs derived from Wösten's model showed promising results for certain localities, such as Cerhovice and Černičí, with an acceptably good fit. However, the estimations for other sites, like Brozany, Ovesná Lhota, Tupadly, Džbánov, Podlesí, and Žichlínek, were less successful due to insufficient input data. Additionally, the authors developed their own pedotransfer functions for sites with adequate data, leading to improved SWRC estimates. In a separate study, Matula et al. (2007) applied Wösten's continuous PTFs to data from Tišice in the Czech Republic. Two types of fitting (4-parameters and 3-parameters) were tested to optimize the parameters of the van Genuchten's equation. Their study showed that continuous PTFs may not be fully suitable for estimating SWRCs in the locality Tišice. However, when the parameters were calculated specifically for each site, the estimates showed better agreement with the measured retention curves.

The creation of the HYPRESCZ database of soil hydrophysical properties in the Czech Republic facilitated the derivation of PTFs for estimating SWRCs (Mihalikova et al., 2013). By employing Wösten's model, the newly derived regression coefficients for the PTFs showed higher reliability compared to the original PTFs, especially for Czech soils. Furthermore, Mihalikova et al. (2014) used the HYPRESCZ database to estimate FC and WP of agricultural land resources on a countrywide scale. They developed class PTFs to estimate FC and WP and combined the results with the Soil Texture Map of the Czech Republic to create new maps of FC and WP for topsoil and subsoil separately.

In another study, Vlček and Hybler (2015) evaluated and compared various pedotransfer functions, both domestic and foreign, for the basic use in agriculture in the Czech Republic. Among the tested PTFs, the ones according to Tomasella and Hodnett (1998) and Batjes (1996) showed the best correlation for field water capacity and wilting point estimation.

Batkova et al. (2022) demonstrated the applicability of recently published PTFs based on a machine learning approach for indirectly determining Ks in the Czech Republic. They compared the performance of these novel PTFs with well-known hierarchical PTFs for 126 soil datasets. The results showed high variability in Ks between and within study areas, especially where preferential flow occurred. In most cases, the tested PTFs overestimated Ks values, particularly for medium to fine-textured soils. Notably, Neural Network analysis PTFs in Rosetta produced the best estimates, showcasing their potential for accurate Ks predictions. In their follow-up study, Báťková et al. (2023) explored the functional evaluation of three publicly available types of PTFs for predicting the Ks. They applied ten PTF models to 56 datasets, including measured Ks values and various predictors. The results revealed substantial variability in Ks within the study field. While the tested PTF models were based on robust soil databases, they showed limited accuracy unless local soil data were incorporated into the PTF development.

The utilization of pedotransfer functions has proven to be a valuable approach for estimating soil hydraulic properties in the Czech Republic, especially when direct measurement data is limited. The continuous development and refinement of these functions hold significant potential for improving the accuracy and efficiency of estimating soil hydrophysical properties, benefiting various agricultural, environmental, and engineering applications.

2. Hypotheses and Objectives

Hypotheses of the thesis are:

Surfactant applications are anticipated to induce significant alterations in various soil properties, encompassing hydraulic conductivity and nutrient distribution. Additionally, it is expected that those applications will influence the soil's nitrification processes, consequently resulting in observable changes in levels of NH_4^+-N and NO_3^--N, impacting the degradation of soil organic matter, potentially instigating discernible shifts within organic carbon fractions.

The utilization of appropriate PTFs to estimate soil hydraulic properties (e.g., field capacity and saturated hydraulic conductivity) can significantly reduce errors and enhance accuracy of the estimated values.

PTFs are adaptable across regions, and their effectiveness in improving decision-making processes in land and water resource management is not limited to specific geographical areas. The consideration of regional variations in soil characteristics when developing and applying PTFs results in more accurate estimations.

The objectives of the thesis are:

1. Analyse the impact of repeated H2Flo applications on soil properties, including water content, hydraulic conductivity, nutrient distribution, organic carbon fractions, and soil nitrification rates, with a focus on NH_4^+-N and NO_3^--N ratios and levels.
2. Investigate shifts in byproducts of organic matter degradation under varying moisture, temperature, and matric potential conditions by investigating different organic carbon fractions (e.g., water-soluble organic carbon, hot water-soluble organic carbon, potassium permanganate oxidizable organic carbon, total organic carbon),
3. Introduce a novel approach to estimate field capacity (FC) by utilizing moisture constants (Retention Water Capacity and Maximum Capillary Water Capacity) and appropriate statistical models,
4. Indirectly determine saturated hydraulic conductivity (Ks) and test the applicability of recently published PTFs based on a machine learning approach, comparing their performance with well-known hierarchical PTFs.

3. Publications

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Implications of surfactant application on soil hydrology, macronutrients, and organic carbon fractions: An integrative field study

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Abstract: This study investigates the effects of repeated applications of the non-ionic soil surfactant H2Flo (ICL-SF Inc., Israel) on the soil water content, hydraulic conductivity, nutrient distribution, and organic carbon fractions (OCFs) in non-hydrophobic loamy sand soils under subsurface drip irrigation. Our results indicate that H2Flo treatment reduces both saturated and unsaturated hydraulic conductivity while promoting the uniform irrigation distribution, consistent with previous findings on surfactants' effects on sandy soils. An increase in soil pH levels, organic carbon content, and extractable magnesium, calcium, and potassium was observed in treated soils, with elevated levels of potassium permanganate oxidizable organic carbon (POXC) implying accelerated decomposition rates. Notably, a positive linear relationship was found between POXC and the increased NO_3^--N content of treated soils, suggesting induced conditions of nitrification. However, the carbon fractions water-soluble organic carbon (C_{ws}) and hot water-soluble organic carbon (C_{hws}) remained quantitatively unchanged, even though they exhibited a positive linear relationship with the soil's hydraulic conductivity. The study highlights the crucial role of monitoring changes in OCFs and nutrient dynamics after surfactant application to optimize soil organic matter utilization and chemical fertilizer management.

Keywords: extractable nutrients; nitrogen sources; hot water-soluble organic carbon; hydraulic conductivity, water-soluble organic carbon

Commercial wetting agents, typically based on alkyl block polymer (ABP) or polyoxyalkylene polymer (PoAP) surfactants, enhance re-wettability and infiltration rates in water-repellent sandy soils (Cisar et al. 2000; Dekker et al. 2005; Oostindie et al. 2008) and augment soil hydration in urban lawns (Dekker et al. 2019). Surfactants, comprised of polar and nonpolar parts, are attracted to the hydrophobic surfaces of soil particles, leading to alterations in both the rate of water infiltration and water distribution within the soil profile (Mobbs et al. 2012). The performance and sustainability of these products can vary significantly, particularly concerning the balance between soil water holding and infiltration abilities (Song et al. 2014), necessitating individual product examinations.

Recently, there has been a noticeable shift in the scientific focus of surfactant research. This change

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is driven by new findings on surfactant-sourced hydrophobicity (Song et al. 2019) and a rise in both dissolved organic carbon (DOC) and particulate organic carbon (POC) in soil leachates after treatment (Song et al. 2018, 2021). Specifically, PoAP-based surfactants have been observed to create hydrophobic layers on sand after multiple applications, transforming even naturally adsorbent sands to resist water. The observed rise in POC in the leachates from these treated soils is believed to indicate surfactants displacing the native organic layers on sand particles. Interestingly, ABP-based products did not induce such a change in either inherently hydrophobic or adsorbent soils in the referenced studies. Yet, a separate study highlighted that ABP-based surfactants diminished microbial activity by effectively stripping organic coatings from the sand grains (Song et al. 2019). In alignment with this, a comprehensive study by Kintl et al. (2022) delved into the impact of various wetting agents on water stable aggregates (WSA). They found a significant decrease in WSA, linked to a reduction in soil organic carbon (SOC).

In addition to the limited understanding of how wetting agents impact soil organic carbon storage, there is also a noticeable lack of studies addressing the dynamics of nutrient availability. A study by Chang et al. (2020) evaluated the effects of surfactant applications on lawns planted with St. Augustine grass (*Stenotaphrum secundatum*). Predictably, there was an enhancement in soil moisture and the quality of the turfgrass. However, the levels of ammonium nitrogen (NH_4^+-N), nitrate nitrogen (NO_3^--N), extractable phosphorus (P), DOC, and total organic carbon (TOC) in the soil leachates remained unchanged. On the plant side, Chaichi et al. (2017) observed enhanced nutrient absorption in tomato plants when treated with a surfactant. In a study by Banks et al. (2015), three commercial surfactants (Activator 90, Agri-Dex, Thrust) were examined. The research showed that the plant potassium (K) uptake was reduced in clay loam soils when treated with Thrust. Conversely, in soils treated with Activator 90 and Agri-Dex, there was a significant decrease in the uptake of several macro- and micro-nutrients.

Despite the poorly understood dynamics of nutrient fixation and release in surfactant-treated soils, the application of surfactants aided in the elimination of specific organic contaminants like polycyclic aromatic hydrocarbons (PAH), enhancing their desorption and fostering their degradation, as noted by Yang et al. (2017) and Li et al. (2019).

H2Flo (ICL-SF Inc., Israel) is a commercial non-ionic PoAP-based soil surfactant. The manufacturer notes that the product contains a minor organic element presented as 'root activator' molecules. This study aims to (*i*) uncover the changes in saturated (K_s) and unsaturated (K(h)) hydraulic conductivity of non-hydrophobic loamy sand soils under subsurface drip irrigation while (*ii*) exploring the induced alterations in nutrient distribution and chemically distinguished organic carbon fractions (OCFs) following applications of the wetting agent H2Flo; (*iii*) magnesium (Mg), calcium (Ca), and extractable phosphorus (P) were examined due to their agronomic significance and their possible modified distribution under surfactant applications; (*iv*) to understand potential shifts in soil nitrification rates due to expectedly altered soil and water interactions, the ratios and levels of NH_4^+-N and NO_3^--N were assessed; (*v*) to further comprehend the shifts in byproducts of organic matter degradation under different conditions of moisture, temperature, and matric potential, we examined the content and distribution of hot water-soluble organic carbon (C_{hws}), water-soluble organic carbon (C_{ws}), potassium permanganate oxidizable organic carbon (POXC), and TOC.

In our study at a specific loamy sand soil locality, we investigate the application of the wetting agent H2Flo, even to naturally non-hydrophobic soils. Loamy sand soil, despite being naturally non-repellent, can benefit from enhanced water residence time in the root zone, especially in regions where this soil type prevails. This approach aligns with our study's objectives, which aim to assess whether OCFs would be influenced in terms of their mobility with modified K_s and K(h) of the soils, as has been previously reported for physically distinguished carbon fractions such as particulate organic carbon or dissolved organic carbon by other studies. Through these monitoring efforts, informed decisions can be made about wetting agent applications and other management practices. This could lead to more efficient nutrient use, increased crop productivity, reduced environmental impacts, and improved soil health and resilience. The present research is anticipated to offer substantial insights into the interplay of water/nutrient adsorption by soil mineral particles when exposed to wetting agent treatments. Additionally, it explores their connections with OCFs, standing out as one of the comprehensive field studies.

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MATERIAL AND METHODS

Description of the study area and soil sampling. The research field is situated in the Benátky nad Jizerou district, Central Bohemian Region, Czech Republic, and features loamy sand soils consisting on average from 81.2% of sand, 13.3% of silt and 5.5% of clay. Positioned at an altitude of 220 m with WGS84 coordinates 50.2782878N, 14.8392344E, the region has a temperate climate marked by gentle, dry winters. The area registers a long-term average temperature of 8.4 °C and an annual rainfall of 560 mm. This site is nestled in the alluvial plains of the Jizera River, notable for its varied soil compositions, predominantly sandy in nature.

Potatoes were sowed on 1 April 2019, with drip irrigation starting on 1 May 2019. Organic fertilizer was applied in spring at a rate of 10 t/ha. Before the planting on 1 April and subsequently on 28 April, just before the canopy took shape, NPK fertilizer was used, amounting to 180 kg N/ha in total. The wetting agent, H2Flo, was dispensed three times through subsurface driplines: on 3 May, 5 June, and early July, with each application consisting of 5 L mixed into 1 000 L of water. From 11 June onward, fungicides and insecticides were used, with subsequent applications every 7–10 days. Before H2Flo applications and after the second application of H2Flo, disturbed soil samples were collected from two depth ranges, 0–15 and 15–30 cm. A detailed depiction of the study area location and sampling scheme is provided in Figure 1A, while a schematic representation of the sensor placement is provided in Figure 1B.

Soil analyses. K_s was determined using undisturbed core rings (250 cm^3) employing a KSAT device (Meter Group Inc., USA), falling head technique. These samples were collected after the initial two applications of H2Flo. The soil had no considerable structure. Four core rings were tested three times each for the control and H2Flo treated soils. For statistical assessment, the obtained K_s values (measured in cm/day at 20 °C) underwent a logarithmic transformation. The naturally wet disturbed samples were carefully mixed and sieved (8 mm) to remove any larger objects, such as stones, roots, and earthworms. The cleaned soil samples were then repacked into containers with a 5 L volume, maintaining a dry bulk density value of 1.44–1.49 g per cm^3 and an initial soil water content of 0.055 g/g. Subsequently, the Mini Disk Infiltrometer (Meter Group Inc., USA) was employed to determine K(h) in these artificially packed soil columns. Repacked soil columns on structureless soil were preferred due to the difficulty of using the infiltrometer in a potato field. Two pressure heads, namely –2 and –5 cm, were consecutively applied during each measurement. The disturbed soil samples were taken after the second application of H2Flo.

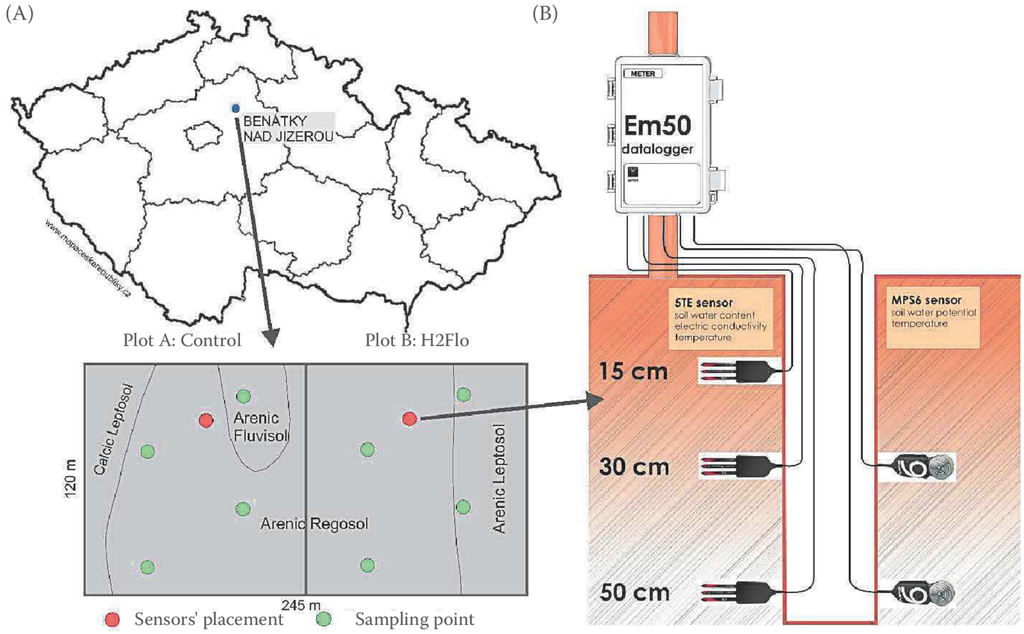

Figure 1. Study area location and sampling scheme (A) and schematic representation of the sensor installation (B)

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The TOC content was determined using the method developed by Nelson and Sommers (1996) based on rapid dichromate oxidation. The electrical conductivity (EC) and pH of the soils were determined in a 1 : 2.5 dH_2O solution (Rayment & Higgenson 1992). Extractable concentrations of Ca, K, Mg, and P were ascertained using the Mehlich III solution method (Mehlich 1984). Concentrations of NH_4^+-N and NO_3^--N were gauged post 0.01 mol/L $CaCl_2$ extraction, as prescribed by ISO 14255:1998. The C_{ws} and C_{hws} levels were identified using a modified Körschens method (Körschens 1980). The POXC measurement followed the method detailed by Weil et al. (2003), which relies on the discernible colourimetric variation at a 540 nm wavelength in 0.2 M $KMnO_4$ soil extracts. Changes in POXC were investigated since it is viewed as a gauge for the readily decomposable carbon reservoir, comprising a mix of both water-repellent and water-attracting compounds, which arise from the preliminary breakdown of soil organic matter (SOM) (Bongiorno et al. 2019). This indicator of labile carbon pool may highlight the altered degradation dynamics after surfactant applications. C_{ws} refers to the fraction of TOC that can dissolve in water at room temperature. These could include simple sugars, amino acids, and certain other organic compounds, which are often readily available for microbial activity and can contribute significantly to soil fertility and nutrient cycling. Conversely, C_{hws} contains a greater variety of complex organic compounds (Uchida et al. 2012). These include microbial biomass carbon, root exudates, amino acids, and carbon linked to soil enzymes (since many enzymes are denatured at high temperatures), which allows C_{hws} analysis to cover significantly more carbon than C_{ws} analysis can. The relevant soil analyses were carried out with three replicates revealing the properties of four sampling points per treatment.

The non-hydrophobic nature of the experimental soil was determined using the standard soil survey test method for water-repellency (Roberts & Carbon 1971; King 1981). Deionized water was dropped onto the surface of both control and treated soils and was observed to be absorbed in under 1 second.

Monitoring the soil water content. The sensors 5TE by METER Group Inc. (USA/Germany) which uses capacitance and thermistor technology to monitor soil's volumetric water content (VWC), bulk EC, and temperature, were used to monitor the relevant parameters. It provides high precision with ±3% VWC accuracy in typical soils and a temperature accuracy of ±1 °C.

The MPS-6 matric potential sensors, from the same manufacturer, were used to monitor the soil water potential. It operates well in drier systems where tensiometer cavitation would be a problem. The MPS-6 covers a range from –10 to –10 000 kPa.

The EM50 data loggers, also by METER Group Inc., were used to collect data from sensors. This five-channel device reads sensors with analogue or digital outputs and is designed for long-term, low-power usage. The monitoring period for data collection using these loggers extended from April 16th to August 15th, 2019. Sensor positions throughout the soil profile are shown in Figure 1B.

Statistical analyses. Statistical evaluations and visualizations were conducted using STATISTICA software (Ver. 13, Statsoft, USA). The normality of the data were checked before variance analysis, per each parameter for the same soil depth and treatment by Shapiro-Wilk test ($P < 0.05$). Differences between treatments and soil depths were assessed using t-test based on groups of control and H2Flo treated soils or soils of 0–15 and 15–30 cm. Pearson's correlation coefficient were used to explain linear relationships between parameters.

Given the nature of saturated hydraulic conductivity data for soils, it is common to observe a wide range of values with an erratic distribution, which commonly directs researchers to log-transform of the data as in the current study. In that context, K_s results were evaluated with both t-test and the F-test and non-parametric Kruskal-Wallis test.

RESULTS AND DISCUSSION

Distribution of soil water content in the root zone. Repeated applications of the H2Flo provided more uniform distribution of soil VWC in the root zone compared to the control soils as observed by 5TE sensor measurements during the monitoring period (Figure 2A, B). Irrigation events are noticeable till the first half of July, when the rainy period occurred and at the end of July the irrigation was terminated. The water content values were in accordance with the observed matric potential differences by MPS-6 sensors (Figure 2C). The influence on soil VWC was more pronounced at 30 and 50 cm depths, along with the 15 cm depth after the second application of H2Flo in June. These findings are consistent with the well-defined improvements that can be provided

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by wetting agent applications in non-hydrophobic soils. Wetting agents, known for their strong affinity for soil surfaces, are adsorbed onto even non-hydrophobic soil particles. Concurrently, this process can enhance water penetration into the soil, regulating the redistribution of water within the soil profile. The application of these agents is well documented for the management of water repellency in thatch and surface layers in sandy soils and for the enhancement of soil hydration (Oostindie et al. 2008; Dekker et al. 2019). Recently, wetting agents have been widely used to homogenize water distribution at the root zone, too (Ou & Latin 2018). In accordance, significant increases in soil water contents after treatment with surfactants have been documented by many researchers (Oostindie et al. 2005; Moore et al. 2010).

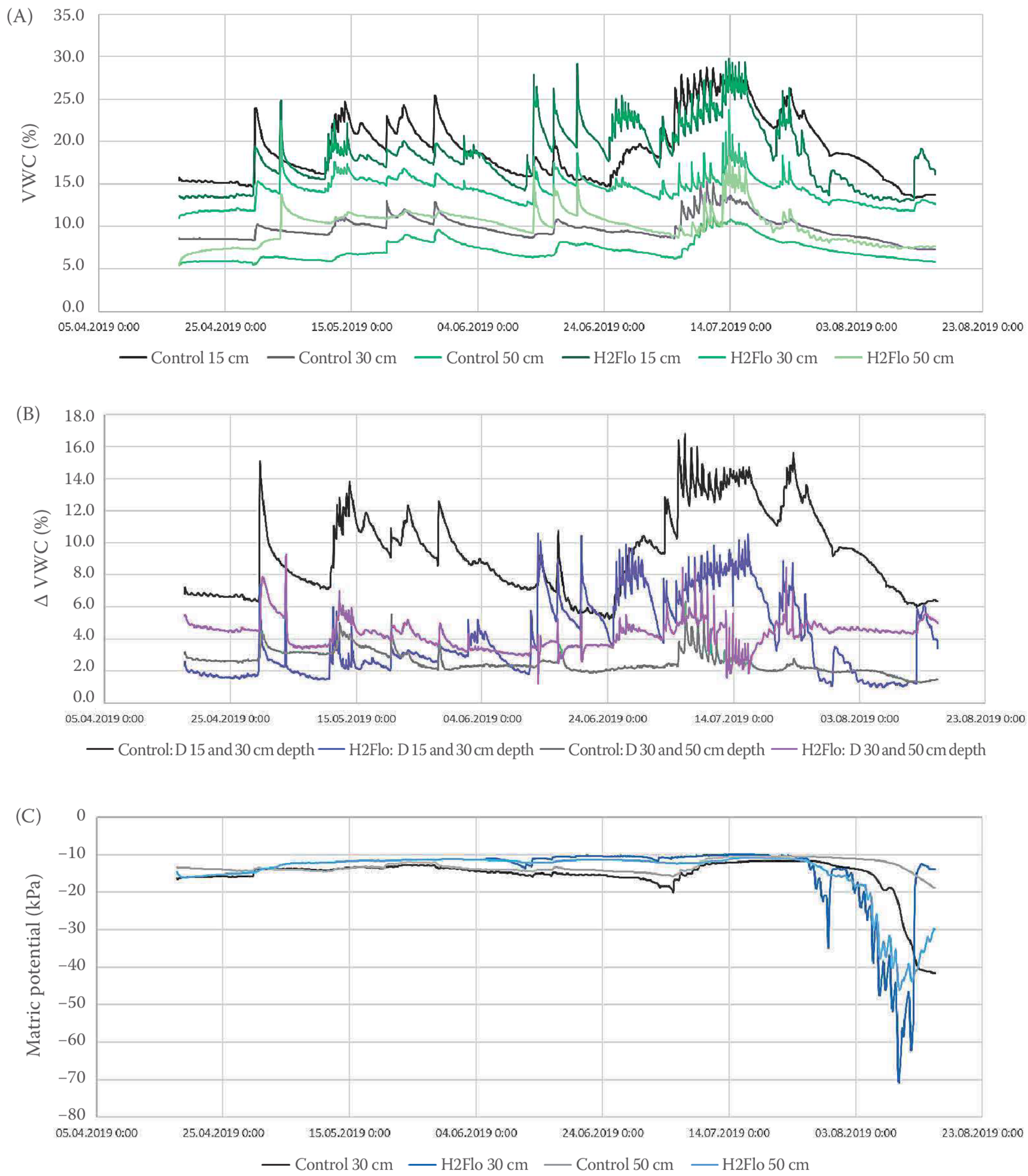

Figure 2. Visualization of the impact of non-ionic soil surfactant H2Flo treatment on soil volumetric water content (VWC) and matric potential: comparison of VWC between untreated control soils and H2Flo treated soils (A); variation in soil water content at different depths for both the control and H2Flo treated soils (B); difference in matric potential values between control and H2Flo treated soils (C)

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Table 1. Statistical evaluation of soil physicochemical properties based on treatments

	Before application of H2Flo				After 2nd application of H2Flo			
Depth (cm)	0–15		15–30		0–15		15–30	
Treatment	H2Flo	control	H2Flo	control	H2Flo	control	H2Flo	control
pH	5.0875	5.2225	5.3325	5.4975	5.215**	4.6675	5.3875*	5.045
EC (µS/cm)	266.25*	149.4	224**	80.525	384.75	492.75*	266.5	301.5
TOC (g/kg)	5.9	7.7	5.9	7.1	10	10	9.6	8.1
SOM[a] (%)	1.02	1.33	1.02	1.23	1.73	1.73	1.66	1.4

H2Flo – non-ionic soil surfactant treated soil; EC – electrical conductivity; TOC – total organic carbon; SOM – soil organic matter; [a]Van Bemmelen transformation of TOC with the factor of 1.724; t-test applied for the soils of the same depth and the same treatment; *,**$P < 0.05$, 0.01

Figure S1 in Electronic Supplementary Material (ESM) presents the lower temperature through the profile of treated soils, as a result of increased VWC values, particularly after the second application of the product, as demonstrated in Figure 2A.

Physicochemical characteristics of the soil. The differences in pH, electrical conductivity, and TOC in soil profile were evaluated by ANOVA before the application of H2Flo to eliminate any potential misunderstanding about possible spatial natural variability. The only significant difference was observed in the electrical conductivity of the soils, which did not affect the salinity interpretation class (Table 1).

Soil reaction was significantly influenced by the surfactant treatment at both soil depths, resulting in slightly elevated pH values. Boomgaard et al. (1987) provided an explanation on the adsorption of non-ionic surfactants. Surfactants are amphiphilic molecules, meaning they have both hydrophilic (water-attracting) and lipophilic (fat-attracting) parts. The primary mechanism for adsorption when the surfactant concentration is low involves hydrogen bonding. This occurs between the non-ionic surfactant chain and the hydroxyl groups located on the mineral surface. As a result of this hydrogen bonding, non-ionic surfactants adsorb in the form of individual units or monomers, leading to a reduced concentration of hydrogen ions and an increase in soil pH.

The difference in electrical conductivity between the soil depths was lower in the treated soils compared to the control soils. This may be connected with a more even distribution of the soluble salts throughout the soil profile as a result of observed changes in VWC throughout the soil profile. The untreated soils exhibited significantly higher EC values at 0–15 cm depth. Contrary to the untreated soils, TOC values were in a similar range for both soil depths in the treated soils, resulting in significantly higher TOC content in the subsoil.

Given the coarse texture of the experimental soils and the region's typical highly acidic pH values, nutrient availability dynamics are of utmost importance in our study.

Extractable macronutrients. In the H2Flo treated topsoils, concentrations of extractable Ca, K, and Mg were markedly elevated (as shown in Figure 3). While Ca and Mg concentrations also increased in the treated soils between 15–30 cm depth, K concentrations did not exhibit significant differences at this depth. Notably, the only discernible variation in nutrient concentrations across depths in control soils

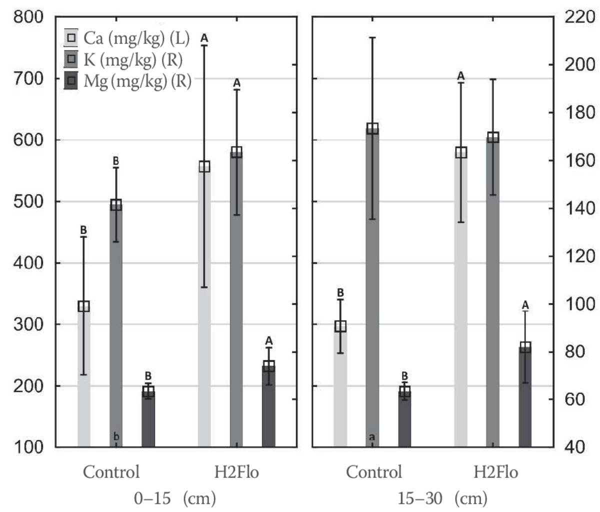

Figure 3. Alterations in extractable Ca, K and Mg levels relative to treatment and soil depth

L – left y-axis; R – right y-axis; H2Flo – non-ionic soil surfactant treated soil; statistically significant differences between treatments at the same sampling depth are denoted by capital letters, while differences between sampling depths are indicated ($P < 0.05$)

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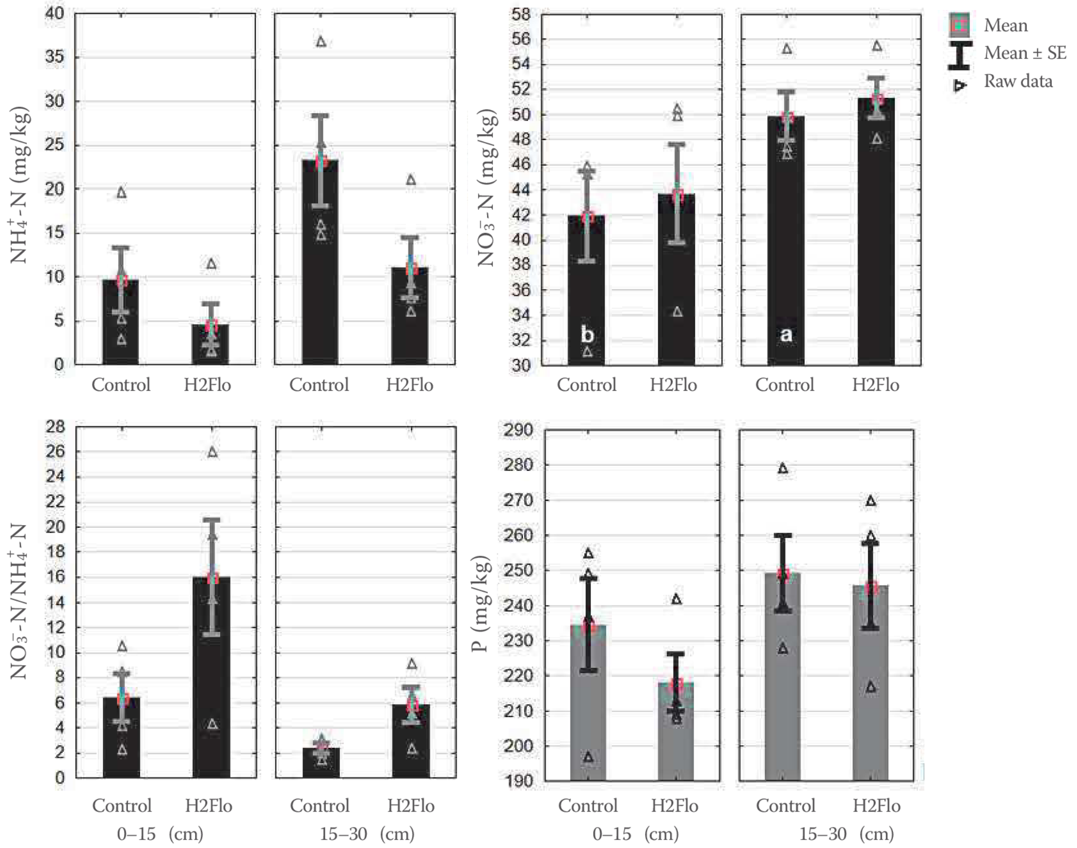

Figure 4. Variations in nitrogen sources, nitrogen source ratios, and extractable P in relation to treatment and sampling depth H2Flo – non-ionic soil surfactant treated soil; statistically significant differences between sampling depths are indicated using lowercase letters within the corresponding columns ($P < 0.05$)

pertained to K content, which manifested substantially higher concentrations at 15–30 cm ($P < 0.05$) relative to the topsoil.

In a recent specialized investigation (Ogunmokun & Wallach 2021), varying doses of a non-ionic surfactant blend (Aquatrols) were administered to grapefruit crops in sandy loam soils supplemented with treated wastewater. As anticipated, both soil moisture levels and the degree of saturation increased. Interestingly, the study reported that the surfactant treatments led to significantly diminished levels of extractable K and exchangeable Ca + Mg at soil depths of 0–20 and 20–40 cm. These reductions were corroborated by the observed decrease in soil electrical conductivity. It is noteworthy that higher crop yields were observed in the treated soils compared to the untreated soils, possibly indicating enhanced nutrient uptake by the plants. This contrasting outcome aligns with the observations of Banks et al. (2015), emphasizing the product-specific ramifications of wetting agents on the availability of soil nutrients.

The rise in the concentrations of extractable nutrients in the current study might be linked to the shift in pH towards a more neutral soil reaction. Notably, the treated soils exhibited a significant rise in pH at both depth intervals, potentially enhancing nutrient availability. Given that EC values were found to decline post-treatment, the elevated pH could be a contributing factor to the noted increase in nutrient concentrations.

Nitrogen sources and extractable phosphorus. Following H2Flo applications, a significant reduction in NH_4^+-N was observed at both soil depths, while NO_3^--N showed a proportionate ascent, as depicted in Figure 4. This points towards an environment favourable for nitrification. Consequently, the most pronounced distinction between treatments manifested in the comparative ratios of these forms of N, with a P-value of 0.057 in the t-test . Chang et al.'s (2020) findings concerning N sources aligned with the subtle significance of our observations. Contrastingly, Ogunmokun and Wallach (2021) documented a decline in total N across both depths.

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In one of the exceptional studies regarding the influence of non-ionic surfactants on the NH_4^+-N and NO_3^--N content of potato-grown sandy loam soils, Arriaga et al. (2009) reported decreased content for both of these nutrients. A significant reduction (30.1%) was observed in soil NO_3^--N concentration 20 days after the final N fertilization when a surfactant was applied, regardless of the N application rates. There was also a trend towards a decrease in soil NH_4^+-N following the surfactant application, though this reduction was less pronounced (19.7%, with a P-value of 0.12).

No significant differences were observed between treatments or depths regarding extractable P concentrations, although they were marginally reduced in the treated soils, as illustrated in Figure 4. These observations align with those reported by Ogunmokun and Wallach (2021) and Chang et al. (2020). It should be emphasized that study of Chang et al. (2020) was confined solely to topsoil examination. Figure S2 in ESM provides insight into the enhanced vegetative growth via crop coverage, enhanced vegetation index (EVI) and normalized difference vegetation index (NDVI) of treated and control soils.

Organic carbon fractions. Repeated applications of H2Flo led to a significant increase in POXC content of topsoils, while the C_{hws} and C_{ws} contents of both top and subsoils remained unchanged (Figure 5). The POXC and C_{hws}, being initial products of SOM degradation, have been identified to have strong associations with the WSA, water holding capacity, and bulk density of soils, as described by Bongiorno et al. (2019). Additionally, these components correlate with extractable forms of N, P, and sulfur (S) as highlighted by Verma et al. (2010). Blair et al. (2006) further noted that K(h) and the average weight diameter of aggregates were linked to POXC changes through inverse and direct relationships, respectively.

The concurrent rise of POXC at both soil depths suggests that the change could primarily stem from distinctly altered degradation conditions—heightened moisture, reduced temperature, and matric potential. The H2Flo treatment's organic input, derived from the product's organic root activator molecules, might play a minor role. Regrettably, specifics regarding the quantity or character of these organic compounds remain elusive. When factoring in the treatment dosage of 5 L of H2Flo per hectare, it is clear that the H2Flo's cumulative contribution cannot solely account for the observed elevation. Additionally, a marked rise in TOC content in the treated subsoils (Table 1) possibly underscores that the POXC fraction might have had a dominant influence on the witnessed growth. This could be attributed to the induced degradation conditions and a more uniform distribution of nutrients and water.

In the control soils, there was a pronounced negative association between POXC and NH_4^+-N (r = –0.983, P = 0.017). Conversely, in the treated soils at depths between 15–30 cm, POXC displayed a marked positive relationship with the NO_3^--N/NH_4^+-N ratio (r = 0.993, P = 0.007). The induced decomposition of SOM after repeated application of wetting agents is a phenomenon that has been particularly noted in previous remediation studies on polycyclic aromatic hydrocarbons such as phenanthrene (Yu et al. 2007) and

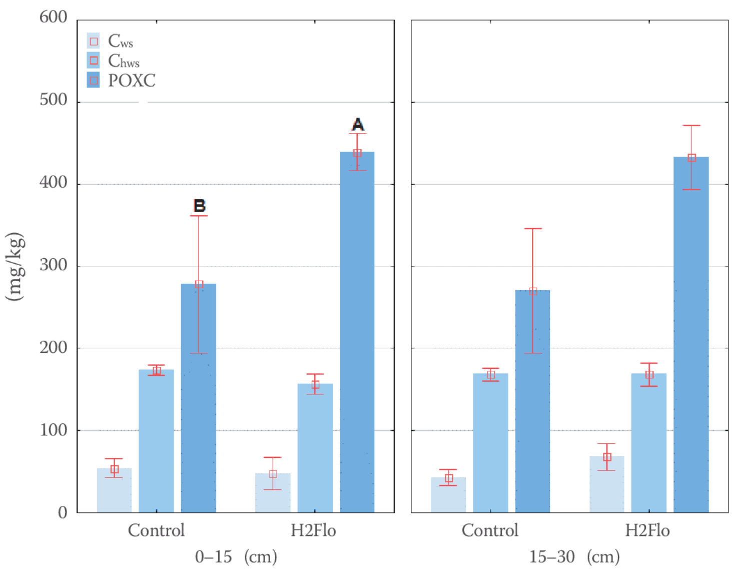

Figure 5. Variations in organic carbon fractions in relation to treatment and sampling depth H2Flo – non-ionic soil surfactant treated soil; C_{ws} – water-soluble organic carbon; C_{hws} – hot water-soluble organic carbon; POXC – potassium permanganate oxidizable organic carbon; statistically significant differences between treatments at the same sampling depth are denoted by capital letters (P < 0.05)

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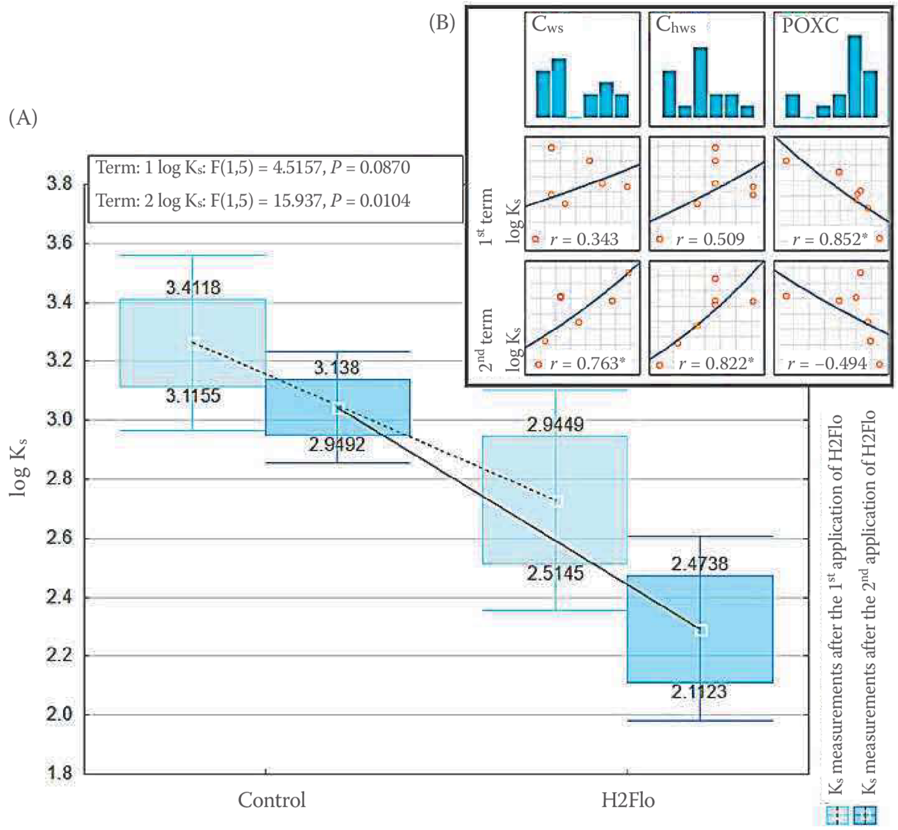

Figure 6. Alterations of saturated hydraulic conductivity (K_s) (log base 10 of cm/day outcomes) of topsoils in response to treatments (A); Pearson correlation coefficients of K_s and OCF in the scatterplots (B)
H2Flo – non-ionic soil surfactant treated soil; C_{ws} – water-soluble organic carbon; C_{hws} – hot water-soluble organic carbon; POXC – potassium permanganate oxidizable organic carbon; $^*P < 0.05$

tributyltin (Mathurasa et al. 2012). Later, Banks et al. (2014) revealed increased microbial activity after non-ionic surfactant applications, with minimal differentiation in microbial community members.

In the H2Flo treated soils, there was a distinct positive association between C_{hws} concentrations and Mg levels ($r = 0.773$, $P = 0.025$). Such relationships between OCF and extractable cations were absent in the control soils. C_{hws} contains various functional groups (like carboxyl and phenolic groups) (Uchida et al. 2012), that can form chelates with metal cations including Mg^{2+}. These chelates can increase the solubility of Mg in soil, making it more readily available for plant uptake.

Soil hydraulic conductivity. H2Flo applications led to a reduction in K_s rates, with the decline being more pronounced after the second application (Figure 6A; $P = 0.01$ in t-test and F-test, $P = 0.03$ in Kruskal-Wallis test). While both treated and control soils exhibited a reduction in rates over time, the variance between the average K_s rates during the sampling intervals was not significant.

In most cases, the decrease is due to: (1) the disintegration of soil aggregates, resulting from the surfactant adhering to minerals and/or the effect of a high sodium adsorption ratio (SAR), which results in pore blockage due to displaced particles (Mingorance et al. 2007; Liu et al. 2022); and (2) the blockage of pores caused by the precipitation of surfactant when divalent cations like Ca^{2+} and Mg^{2+} are present in the soil (Çelik et al. 1978; Stellner & Scamehorn 1986). Additionally, the clay content of the soil is influential in terms of the expansion of minerals and fine particle mobilization (Peng et al. 2017). These changes typically occur after multiple applications rather than when the non-ionic surfactants are initially applied. This is because the initial applications usually result in increased K_s values, particularly in hydrophobic soils.

Considering the increased POXC and nitrification activity, bioclogging could also be a possible factor behind decreased K_s rates. Research has shown that

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bioclogging can result in a decrease in K_s (Hallett & Young 1999). When bacteria colonize soils, they cover the pore walls with biofilms, comprising cells tightly entwined in a network of exopolymer glycocalyx. This causes a reduction in pore space available for water flow and the exopolymer might also lead to alterations in soil swelling properties and dispersion of colloidal particles (Peng et al. 2017).

Some implications are drawn from relatively old studies since the current scientific approach typically deals with K(h) in their experimental designs. The observed decline in K_s values from our study aligns with results from the K(h) tests conducted in laboratory settings using soils from the same region, both treated and untreated (Figure 7). Similar outcomes have been highlighted in various studies over the past two decades, particularly in non-hydrophobic soils (Mobbs et al. 2012; Bashir et al. 2020). Notably, Bashir et al. (2020) associated reduced hydraulic conductivity with a slowed vertical movement and increased lateral dispersion of water and surfactant. When examining potential interplays between K_s and OCFs, existing literature does not offer a direct comparative scenario. This might be due to many studies focusing on K(h) in tandem with DOC or POC, rather than specifically on K_s. Nevertheless, our data points to moderate to robust, yet divergent correlative links between OCFs and K_s, as illustrated in Figure 6B. Specifically, water-soluble fractions revealed a positive association with K_s, whereas POXC displayed an inverse relationship with K_s. Even though the K_s were in positive relationship with C_{ws} and C_{hws}, and negative relationship with POXC, it should be noted that the treated soils were not found to present hydrophobic properties in water droplet test, after applications of H2Flo.

CONCLUSION

Upon repeated application, the non-ionic surfactant H2Flo facilitates uniform distribution of irrigation water throughout loamy sand soil and leads to a reduction in both saturated and unsaturated hydraulic conductivity. This is consistent with the well-documented impacts of non-ionic surfactants on sandy soils.

In the treated soils, pH levels and the distribution of organic carbon content were observed to increase, notably within subsoils. The levels of POXC also rose in the treated soils, a marker for augmented active carbon content, suggesting an accelerated rate of decomposition influenced by changes in water content and distribution. A significant positive correlation was found between POXC and NO_3^--N content, and a negative correlation with NH_4^+-N content, indicative of increased nitrification. NO_3^--N of the treated soils, in this context, was considerably higher compared to the control soils.

Though the carbon fractions C_{ws} and C_{hws} remained quantitatively unchanged post-H2Flo application, they showed positive linear relationships with the soil's hydraulic conductivity and extractable Mg content found in treated soils. Treated soils additionally demonstrated increased levels of extractable Ca and K, likely a consequence of the elevated pH and the increase in organic exchange complexes stemming from higher POXC values. Interestingly, potassium leaching was less pronounced in H2Flo treated soils.

This study elucidates the effects of H2Flo applications, highlighting alterations in SOM degradation products and nitrification dynamics, as well as modifications in the soil's extractable macronutrients. Particularly, the observed changes in OCFs and in the rate of NH_4^+-N to NO_3^--N underscore the importance of meticulous monitoring of these

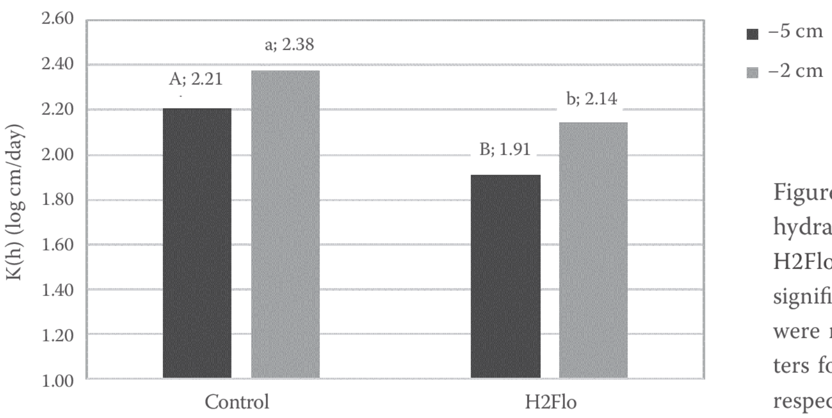

Figure 7. Comparison of average unsaturated hydraulic conductivity K(h)
H2Flo – non-ionic soil surfactant treated soil; significant differences between infiltration rates were represented with low case and capital letters for –2 and –5 cm pressure heads adjusted, respectively; $P < 0.01$

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fractions after surfactant applications, ensuring the sustained advantages derived from organic amendments and nitrogen fertilizers.

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Article

Simple and Cost-Effective Method for Reliable Indirect Determination of Field Capacity

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Abstract: This study introduces a simple and cost-effective method for the indirect determination of field capacity (FC) in soil, a critical parameter for soil hydrology and environmental modeling. The relationships between FC and soil moisture constants, specifically maximum capillary water capacity (MCWC) and retention water capacity (RWC), were established using undisturbed soil core samples analyzed via the pressure plate method and the "filter paper draining method". The aim was to reduce the time and costs associated with traditional FC measurement methods, as well as allowing for the use of legacy databases containing MCWC and RWC values. The results revealed the substantial potential of the "filter paper draining method" as a promising approach for indirect FC determination. FC determined as soil water content at −33 kPa can be effectively approximated by the equation FC33 = 1.0802 RWC − 0.0688 (with RMSE = 0.045 cm^3/cm^3 and R = 0.953). FC determined as soil water content at −5 or −10 kPa can be effectively approximated by both equations FC5 = 1.0146 MCWC − 0.0163 (with RMSE = 0.027 cm^3/cm^3 and R = 0.961) and FC10 = 1.0152 MCWC − 0.0275 (with RMSE = 0.033 cm^3/cm^3 and R = 0.958), respectively. Historical pedotransfer functions by Brežný and Váša relating FC to fine particle size fraction were also evaluated for practical application, and according to the results, they cannot be recommended for use.

Keywords: field capacity; maximum capillary water capacity; retention water capacity; pedotransfer functions; filter paper draining method

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1. Introduction

Field capacity (FC) or field water capacity is defined as the maximum amount of water soil can hold against the force of gravity after excess water has drained away [1,2]. Despite this vague definition, FC is a crucial value for effective soil water management, crop growth, soil health and environmental conservation in agriculture and land management practices. It is a vital input parameter for environmental modeling, particularly in soil hydrology. It serves as a fundamental starting point for simulating water movement, infiltration and runoff in terrestrial ecosystems. Incorporating accurate FC values into models helps researchers and policy makers to predict and manage various environmental processes, such as watershed hydrology, groundwater recharge, flood risk assessment, irrigation and ecosystem health assessment. By providing a basic understanding of how much water the soil can retain, FC data enhance the precision and reliability of environmental models, facilitating informed decision making for sustainable land and water resource management.

Traditional in-situ determination of FC assumes soil, which is deep and permeable, without influence of the groundwater table, with no evaporation from the soil surface. The well-drained soil receives a sufficient amount of water, and after redistribution, the drainage rate decreases rapidly and becomes negligible within about 24 to 72 h. Water is drained from the large non-capillary pores and is now retained in the capillary pores. The fundamental problem is to define this negligibility, as it is a dynamic process [2]. The same authors state that there is no good alternative to the in situ method for the determination of FC. However, it is possible to determine FC from long-term field observations of soil water content and suction pressure [3].

For practical applications and comparability, the complicated in situ process of FC determination has been replaced by laboratory measurements performed on soil core samples. FC is determined as the water content of the soil equilibrated at a specific suction pressure value. The FC value varies with the dynamic properties of the soil profile, such as the hydraulic gradient, hysteresis, stratification of the soil profile, swelling and shrinkage, or the presence of an impermeable layer or a high groundwater table. Therefore, the suction pressure value for this water content cannot be generally defined, especially when a sample is taken and the hydraulic context of the soil is interrupted. However, for calculations and estimates, it is important to associate the FC with some suction pressure value. Coarse-textured soils reach conditions defined as an FC of around −5 or −10 kPa, medium-textured soils at −33 kPa and fine-textured soils at −50 kPa [2]. Therefore, the selected suction pressure level should always be recognized according to the studied soil. In spite of this, the basic concept is often ignored and water content at a suction pressure of −33 kPa is adopted as the most widely used value associated with FC.

The methods of a sand/kaolin box, temp cell [4] and pressure plate apparatus [5] are the most widely used, although they are rather time- and energy-consuming, and therefore costly. Measurements can take several weeks to months, depending on the soil type and the number of points on the soil water retention curve (SWRC) that need to be determined sequentially. It is likely that at least the permanent wilting point (WP) will be determined in addition to FC [6–8] if the full range of SWRC is not required. A modern and relatively fast method is the evaporation method [9], which is utilized, e.g., in the commercial instrument HYPROP (METER Group Inc., Pullman, WA 99163, USA). It can determine the FC within several days, but it is rather costly and requires regular attention, especially in its preparation for use.

Besides the methods mentioned above for the accurate determination of soil matric potential, there are cost-effective alternatives involving filter paper. In the in-contact filter paper technique, initially dry filter paper absorbs liquid water from the soil until equilibrium is reached. Good contact between the filter paper and the soil is essential. After equilibrium, the water content of the filter paper is measured, and the soil suction is estimated using a calibration curve [10,11].

A different method employing filter paper was developed in Central Europe to assess soil water retention properties. Instead of assessing the water content of the moist filter paper, this method involves determining the gravimetric soil water content of core samples. These samples are allowed to drain naturally on the filter paper for a specified period of time [12]. This "filter paper draining method" is used in this study and is further described, specifically regarding the maximum capillary water capacity (MCWC) and retention water capacity (RWC), which have a long history of use in the Czech Republic as an approximation of FC [12–14].

As an alternative to direct measurement, there is an estimation approach utilizing pedotransfer functions (PTFs). PTFs estimate a required soil property that is difficult to obtain (estimand), in this case, FC, from other easily obtainable soil properties (called predictors), typically soil texture, dry bulk density and organic matter content. PTFs employ a wide range of methods from linear regression equations to artificial neural networks, non-parametric algorithms and machine learning approaches [7,8,15–18]. The reliability of PTFs greatly varies and their general applicability may be limited. In any case, for accurate prediction, a database with measured predictors and estimands is needed. However, often, accurate information is not required and a value with higher uncertainty may be sufficient if it can be obtained quickly and at minimal cost.

Efforts to develop statistical relationships between predictors and soil moisture constants were undertaken long before the term PTFs was introduced [2]. It should be noted that the word "constant" can be misleading as it implies invariant behavior of the soil pore system. In Central Europe, regression equations for estimating FC and WP from a fine particle size fraction (FPSF; soil particles < 0.01 mm) have been established [13] and are still in use [19,20]. Although there are different varieties of PTFs for estimating the soil water retention curve or just its important points, such as FC and WP [15–18], they are rarely used by researchers and decision makers for practical applications. FC and WP often need to be determined or estimated for irrigation management purposes or for the quantification of available water capacity [21]. It appears that ease of use is the primary criterion for the practical application of PTFs.

The aim of this study was to investigate the relationship between FC, determined as the gravimetric water content at a given set suction pressure level, and the soil moisture constants "retention water capacity" (RWC) and "maximum capillary water capacity" (MCWC), which can be obtained using the rapid and inexpensive filter paper draining method. These relationships have been developed with the goal of becoming commonly used formulae for the rapid and relatively reliable estimation of FC and, to the present knowledge of the authors, such relationships have not been published yet.

Additionally, simple regression equations according to Brežný and Váša [13] relating FC to the fine particle size fraction (soil particles < 0.01 mm) were tested in this study.

2. Materials and Methods

2.1. Filter Paper Draining Method

The full procedure for processing an undisturbed soil core sample is described in detail including illustrative schemes in Spasić et al. [12]. Only relevant parts of the methodology are presented here.

When the undisturbed soil samples (100 cm^3) were brought to the laboratory, their capillary saturation was the first step. After achieving capillary saturation and recording the initial weight for calculating the saturated water content, water drainage was initiated using folded dry filter paper. Saturated samples were placed under a hood on four layers of dry filter paper for exactly 30 min—precise timing was crucial. The weight was then recorded (not relevant to this study). The initial drainage for 30 min primarily addressed non-capillary pores. The samples were then transferred to four new and dry layers of filter paper under the hood for a further 90 min (2 h in total). The weight recorded at this stage was used to calculate the soil moisture constant MCWC. The wet filter paper was again replaced, and the samples were allowed to drain under the hood for a further 22 h (a total of 24 h) before being weighed to determine the soil moisture constant RWC. Standard qualitative filter paper 2R/80 in sheets cut to 30x35 cm was used, with up to 12 samples placed on this size of filter paper. Each ring was covered with a watch glass during the draining process.

After draining them on filter paper, the samples were transferred to pressure plate apparatus [5] for FC and WP determination (suction pressures of −33 and −1500 kPa, respectively). This step is not part of the filter paper draining method; however, it was included for the purpose of this study in order to compare the soil moisture constants obtained via the filter paper draining method with the FC determined as water content at −33 kPa. The final step was drying in an oven at 105 °C to a constant weight (usually 24 h). After cooling the samples in a desiccator, the weights of the dry samples were determined and the volumetric water contents of all relevant soil moisture constants were calculated via a gravimetric method. A graphical overview of the methodological steps is depicted in Figure 1. In addition, dry bulk density (BD; g/cm^3) was calculated from the dry soil weight and the volume of the ring.

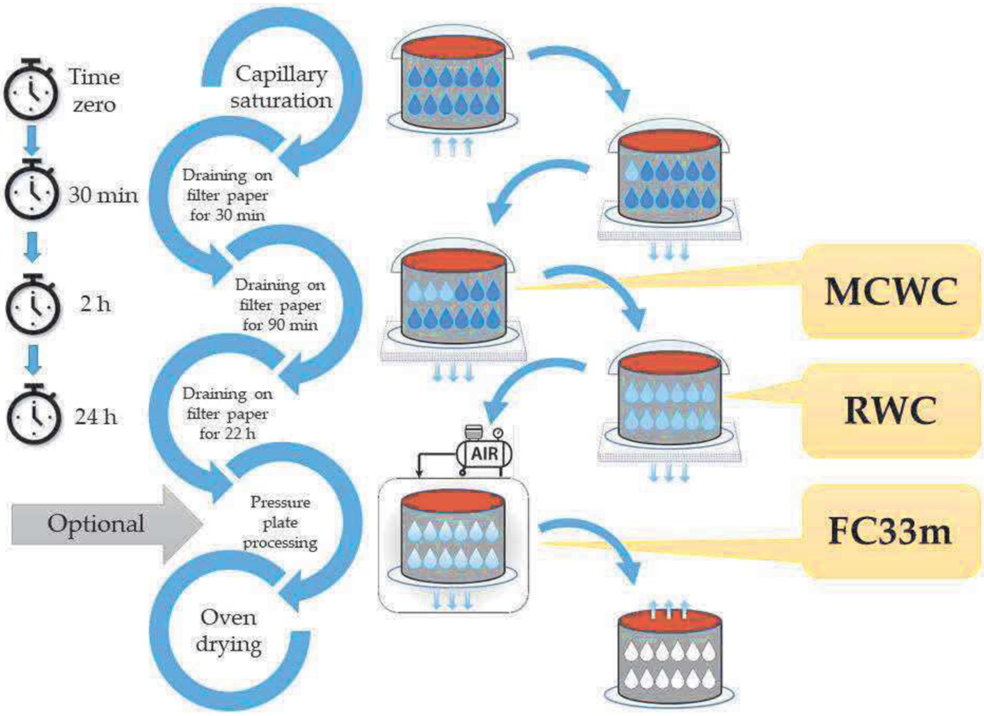


Figure 1. Schematic diagram of the workflow, including filter paper draining method followed by the pressure plate method. MCWC—maximum capillary water capacity, RWC—retention water capacity, FC33m—field capacity measured as water content at −33 kPa.

2.2. Data Origin and Processing

In total, 1212 database entries and/or soil samples from the Czech Republic containing the required information on FC indirect determination were utilized in this study. The total number consisted of three independent sets of data; datasets one and two were used for developing the statistical relationships between FC and MCWC/RWC, while dataset three was used for testing the existing regression equations according to Brežný and Váša [13] for FC estimation. The datasets originated from two sources: (i) the Database of Soil Hydrophysical Properties in the Czech Republic called HYPRESCZ, from which datasets one and three were derived, and (ii) dataset two, containing data on soil samples measured by the authors of this study. The availability and use of data from each dataset are further summarized in Table 1.

Table 1. Summary of data availability within the three datasets.

	Dataset One	Dataset Two	Dataset Three
Origin of data	HYPRESCZ	Measured	HYPRESCZ
N. of data	534	207	471
Purpose of use	To correlate MCWC with FC5f, FC10f, FC33f and FC50f	To correlate MCWC and RWC with FC33m	To test historical PTFs
Availability within the dataset			
MCWC	Yes	Yes	Not relevant
RWC	No	Yes	Not relevant
FC fitted for −5, −10, −33 and −50 kPa	Yes	No	Yes
FC measured for −33 kPa	No	Yes	No
FPSF	Not relevant	Not relevant	Yes

MCWC—maximum capillary water capacity, RWC—retention water capacity, FC—field capacity, 5, 10, 33, 50—suction pressure (kPa, in abs. value), f—fitted, m—measured, FPSF—fine particle size fraction, PTFs—pedotransfer functions.

2.2.1. Dataset One

In the HYPRESCZ database [22], 534 entries containing both measured SWRC and the moisture constant MCWC determined using the filter paper draining method were found. Unfortunately, RWC data were not collected within the database. Suitable data for dataset one originated from 23 different localities, including surface and deeper soil horizons. The database contains data from different sources, and SWRCs were obtained via various methods. For unification, SWRCs were carefully fitted using the van Genuchten Equation (1) [23], as the water retention equilibrium points were obtained at different suction pressures. Each fitted curve was subjected to a careful assessment of the quality of the optimisation to ensure that it represented the measured data well. Further details on the data, including using the RETC code [24] for fitting the SWRC, are provided in Miháliková et al. [22].

$$(\theta - \theta_r)/(\theta_s - \theta_r) = 1/(1 + (\alpha|h|)^n)^{(1-1/n)} \tag{1}$$

where θ is actual water content, θ_r and θ_s are model parameters expressing the residual and saturated soil water contents, respectively (cm^3/cm^3), α and n are shape factors, and $|h|$ is the absolute value of the actual pressure head (cm).

Using the van Genuchten parameters, FC was calculated as the volumetric water content at four different suction pressures associated with FC as listed by Cassel and Nielsen [2]: −5, −10, −33 and −50 kPa. The resulting values of the fitted field capacity were denoted as FC5f, FC10f, FC33f and FC50f, respectively. Their statistical relationships with the measured MCWC values were investigated.

2.2.2. Dataset Two

The second dataset contains 207 undisturbed soil samples (100 cm^3) and it was part of the dataset used for mapping the RWC of soils in the Czech Republic, which is provided as a public service by the Research Institute for Soil and Water Conservation, Prague, CZ, on the website https://mapy.vumop.cz/ (accessed on 1 September 2023). Samples were collected from the surface layer at about 100 different localities covering representative arable lands of the Czech Republic. More detailed information on the data can be found in the study by Vopravil et al. [14]. Soil moisture constants MCWC and RWC were determined using the filter paper draining method as described above prior to the determination of FC using the pressure plate method [5], and defined as the volumetric water content at a suction pressure of −33 kPa (further denoted as FC33m). The suction pressure of −33 kPa was selected based on textural analysis of the sampled soils. In total, 75% of the soils were medium-textured, specifically the loam, sandy loam and silt loam texture classes (USDA).

The statistical relationships of both MCWC and RWC with FC33m were investigated. This relatively large data set is unique in that the data were collected by the same team of researchers and processed in the same laboratory using identical methodologies and equipment. This substantially reduced the error rate associated with the varying treatment of samples, a common challenge in large data collections.

2.2.3. Dataset Three

The last dataset was again retrieved from the HYPRESCZ database, and it contains 471 relevant entries with available FPSF values and fitted van Genuchten parameters of the SWRC. Some entries may overlap with the first dataset; however, the database contains in total more than 2000 entries on arable land, which are fragmented and of varying completeness levels. Thus, all suitable data were used. On the third dataset, the regression functions, which can be considered historically as the first PTFs in the Czech Republic, were tested. These functions have been widely used, as will be further discussed. The functions are denoted as FC by Brežný (Equation (2)) [25] and FC by Váša (Equation (3)) [13].

$$\text{FC by Brežný} = 6.66 + 1.03\ \text{FPSF} - 0.008\ \text{FPSF}^2 \quad (2)$$

$$\text{FC by Váša} = (\text{FPSF} + 18) \times 20)^{0.5} \quad (3)$$

where FC is field capacity in % by volume, and FPSF is content of fine particle size fraction, which are soil particles < 0.01 mm (%).

2.3. Statistical Evaluation and Uncertainty Analysis

Data were processed in MS Excel, including statistical evaluation. Uncertainty analysis was carried out by employing the correlation coefficient (R), coefficient of determination (R^2), mean absolute error (MAE) and root mean squared error (RMSE) to assess the quality of the findings and to foster their transparency and reliability. Equations (4) and (5) represent the latter two statistical indicators:

$$\text{MAE} = \Sigma \mid x_i - x \mid N^{-1} \quad (4)$$

$$\text{RMSE} = [\Sigma(x_i - x)^2\ N^{-1}]^{0.5} \quad (5)$$

where x and x_i represent the observed and predicted values for each data pair i, and N is the total number of observed data pairs.

Higher R and R^2 values were indicative of a stronger linear relationship and better agreement between the observed variables. Conversely, lower MAE and RMSE values signified smaller discrepancies between the observed variables, reflecting a higher level of accuracy in the predictions. It is crucial to utilize several statistical indicators when assessing the quality of statistical relationships. For example, relying solely on a high R can be misleading, as it may suggest a strong linear relationship between two sets of data, while other errors and discrepancies may remain unaccounted for. The R^2 complements the R by providing insight into the proportion of variation in the observations that is explained by the predictions. Meanwhile, MAE and RMSE provide valuable information about the size and distribution of errors in the predictions. These two metrics help to identify situations where predictions, despite a seemingly strong R, may exhibit substantial deviations from the observed values. By combining these four indicators, a more comprehensive assessment of the reliability of the predictions can be obtained. This leads to improving the usefulness of the findings in practical applications and a good reflection of reality [26].

3. Results

3.1. Descriptive Statistics of Soil Properties in the Datasets

The results obtained from the statistical analysis of three distinct datasets, facilitating a comprehensive understanding of the investigated soil moisture characteristics, are presented in this section.

Table 2 offers an insight into the data derived from the HYPRESCZ database (dataset one). This dataset, which was used for investigating MCWC, includes a number of crucial soil properties, including the percentage of clay, silt and sand; dry bulk density (BD); organic matter content (OM); porosity, MCWC; and FC values fitted at four different suction pressures. An illustrative representation of filling the pores with water is summarized through box plots in Figure 2a. Higher values of the coefficient of variation for soil texture or organic matter indicate that there are different soils in the database, covering the high variability of the soils in the Czech Republic.

Table 2. Descriptive statistics of data from HYPRESCZ database for MCWC investigation (dataset one).

Variable	Mean	Minimum	Maximum	Lower Quartile	Upper Quartile	SD	CV
Clay (%)	25.4	3.4	66.9	14.9	34.1	12.5	49.0
Silt (%)	39.3	4.2	73.0	29.3	51.2	14.6	37.1
Sand (%)	35.3	1.0	89.8	23.6	47.6	18.1	51.3
BD (g/cm^3)	1.499	0.800	1.920	1.380	1.660	0.215	14.4
OM (%)	1.226	0.000	14.210	0.330	1.700	1.441	117.5
Porosity	0.4356	0.2558	0.6656	0.3822	0.4818	0.0773	17.8
MCWC (cm^3/cm^3)	0.3807	0.1370	0.6364	0.3290	0.4315	0.0836	22.0
FC5f (cm^3/cm^3)	0.3700	0.0818	0.6368	0.3166	0.4198	0.0883	23.9
FC10f (cm^3/cm^3)	0.3590	0.0733	0.6296	0.3029	0.4099	0.0886	24.7
FC33f (cm^3/cm^3)	0.3371	0.0548	0.6049	0.2852	0.3907	0.0877	26.0
FC50f (cm^3/cm^3)	0.3288	0.0489	0.6047	0.2738	0.3814	0.0873	26.6

BD—dry bulk density; OM—organic matter; MCWC—maximum capillary water capacity; FC—field capacity; 5, 10, 33, 50—suction pressure (kPa, in abs. value); f—fitted; SD—standard deviation; CV—coefficient of variation (%).

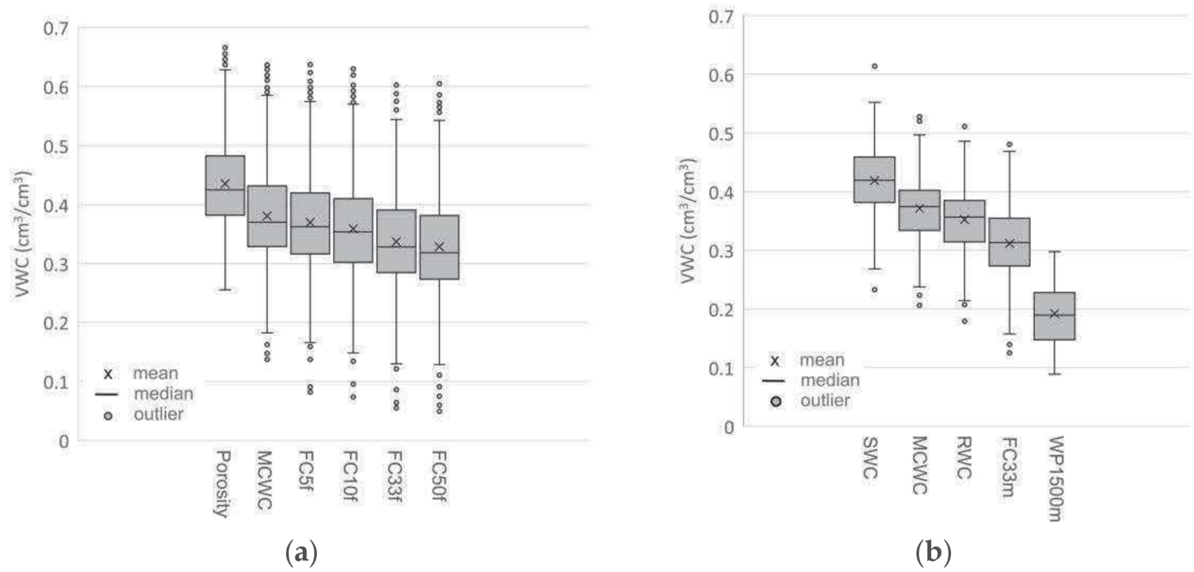


Figure 2. Soil moisture constants: (**a**) dataset one: data for MCWC investigation, (**b**) dataset two: data for RWC investigation. SWC—saturated water content; MCWC—maximum capillary water capacity; RWC—retention water capacity; FC—field capacity; 5, 10, 33, 50—suction pressure (kPa, in abs. value); f—fitted; m—measured; WP1500m—permanent wilting point measured as water content at −1500 kPa. The box—lower and upper quartiles; median—the line splitting the box into two parts; the cross—the mean value; whiskers—minimum and maximum (limited to a maximum of 1.5 times the interquartile range).

The descriptive statistics of dataset two, shown in Table 3, provide insight into the data relating to the investigation of RWC. This dataset consists of soil properties such as saturated water content, MCWC, RWC, FC measured at −33 kPa (FC33m), WP measured at −1500 kPa (WP1500m), and BD. To complement these statistics, Figure 2b provides box plots to visually represent the distribution and variability of soil moisture constants.

Table 3. Descriptive statistics of data measured for RWC investigation (dataset two).

Variable	Mean	Minimum	Maximum	Lower Quartile	Upper Quartile	SD	CV
Clay (%)	18.1	3.9	50.5	11.1	23.5	8.7	48.1
Silt (%)	39.6	4.7	70.1	27.3	51.5	15.1	38.3
Sand (%)	42.3	4.6	91.4	26.1	59.1	20.5	48.6
BD (g/cm^3)	1.480	1.085	1.806	1.369	1.599	0.159	10.7
OM (%)	1.851	0.207	5.293	1.155	2.431	0.941	50.9
SWC (cm^3/cm^3)	0.4189	0.2330	0.6140	0.3814	0.4590	0.0560	13.4
MCWC (cm^3/cm^3)	0.3715	0.2063	0.5278	0.3339	0.4022	0.0526	14.2
RWC (cm^3/cm^3)	0.3525	0.1792	0.5113	0.3145	0.3850	0.0545	15.5
FC33m (cm^3/cm^3)	0.3119	0.1251	0.4805	0.2733	0.3547	0.0617	19.8
WP1500m (cm^3/cm^3)	0.1749	0.0499	0.4104	0.1265	0.2191	0.0667	38.1

BD—dry bulk density, OM—organic matter, SWC—saturated water content, MCWC—maximum capillary water capacity, RWC—retention water capacity, FC33m—field capacity measured as water content at −33 kPa, WP1500m—permanent wilting point measured as water content at −1500 kPa, BD—dry bulk density, SD—standard deviation, CV—coefficient of variation (%).

Furthermore, the descriptive statistics for dataset three are provided in Table 4. Besides the standard texture fractions of clay (<0.002 mm), silt (0.002–0.05 mm) and sand (0.05–2.0 mm), the FPSF (<0.01 mm) is provided, because it is a predictor of Equations (2) and (3). These statistics offer a comprehensive view of the variability exhibited by these soil properties.

Table 4. Descriptive statistics of data from HYPRESCZ database for testing of historical PTFs (dataset three).

Variable	Mean	Minimum	Maximum	Lower Quartile	Upper Quartile	SD	CV
Clay (%)	15.8	0.0	42.8	8.5	19.8	10.4	65.5
Silt (%)	29.4	1.5	70.6	16.8	40.2	15.7	53.4
Sand (%)	54.7	3.6	98.0	37.3	71.2	23.0	42.0
FPSF (%)	27.2	0.4	66.0	16.8	36.2	14.1	51.9
BD (g/cm^3)	1.504	0.991	1.870	1.400	1.620	0.161	10.7
OM (%)	1.427	0.069	12.723	0.414	2.300	1.372	96.1
SWC (cm^3/cm^3)	0.4019	0.2530	0.5914	0.3631	0.4340	0.0578	14.4
FC33f (cm^3/cm^3)	0.2661	0.0567	0.4537	0.2164	0.3242	7.94	29.8
WP1500f (cm^3/cm^3)	0.1513	0.0157	0.3472	0.0996	0.1956	6.82	45.1

FPSF—fine particle size fraction, BD—bulk density, OM—organic matter, SWC—saturated water content, FC33f—field capacity fitted as water content at −33 kPa, WP1500f—permanent wilting point fitted as water content at −1500 kPa, SD—standard deviation, CV—coefficient of variation (%).

3.2. Predictive Relationships between Soil Moisture Constants and Field Capacity

- Maximum Capillary Water Capacity (Dataset One):

MCWC exhibits a strong correlation with FC5f, FC10f, FC33f and FC50f in dataset one (see Figure 3 and Table 5). These correlations have high R and R^2 values, indicating a robust linear relationship between MCWC and the fitted field capacity values at different suction pressures. The RMSE and MAE values for MCWC in relation to FC5f, FC10f, FC33f and FC50f are relatively low, indicating accurate predictions. This suggests that MCWC is a reliable predictor for estimating field capacity in this dataset.

Confidence intervals (0.95) providing a view into the uncertainty when estimating the mean are included in the graphs, along with prediction intervals accounting for variation in the dependent variable around the mean.

It appears that the correlation between MCWC and FC5f stands out as the most favorable (Figure 3a). This correlation exhibits the lowest RMSE and MAE values, signifying smaller discrepancies between the observed and predicted values. It demonstrates the highest R and R^2 values, indicating a strong linear relationship and better agreement between MCWC and FC5f.

- Retention Water Capacity (Dataset Two):

FC33m exhibits a strong correlation with both RWC and MCWC in dataset two (Figure 4). These correlations have high R and R^2 values, implying a robust linear relationship. The RMSE and MAE values for FC33m in relation to RWC and MCWC are relatively low, indicating accurate predictions. This suggests that both retention water capacity and maximum capillary water capacity are reliable indicators for predicting FC at −33 kPa. Based on the uncertainty analysis values (Table 5), it appears that FC33m vs. RWC has better performance, indicating that it may be a more accurate predictor of FC compared to MCWC.

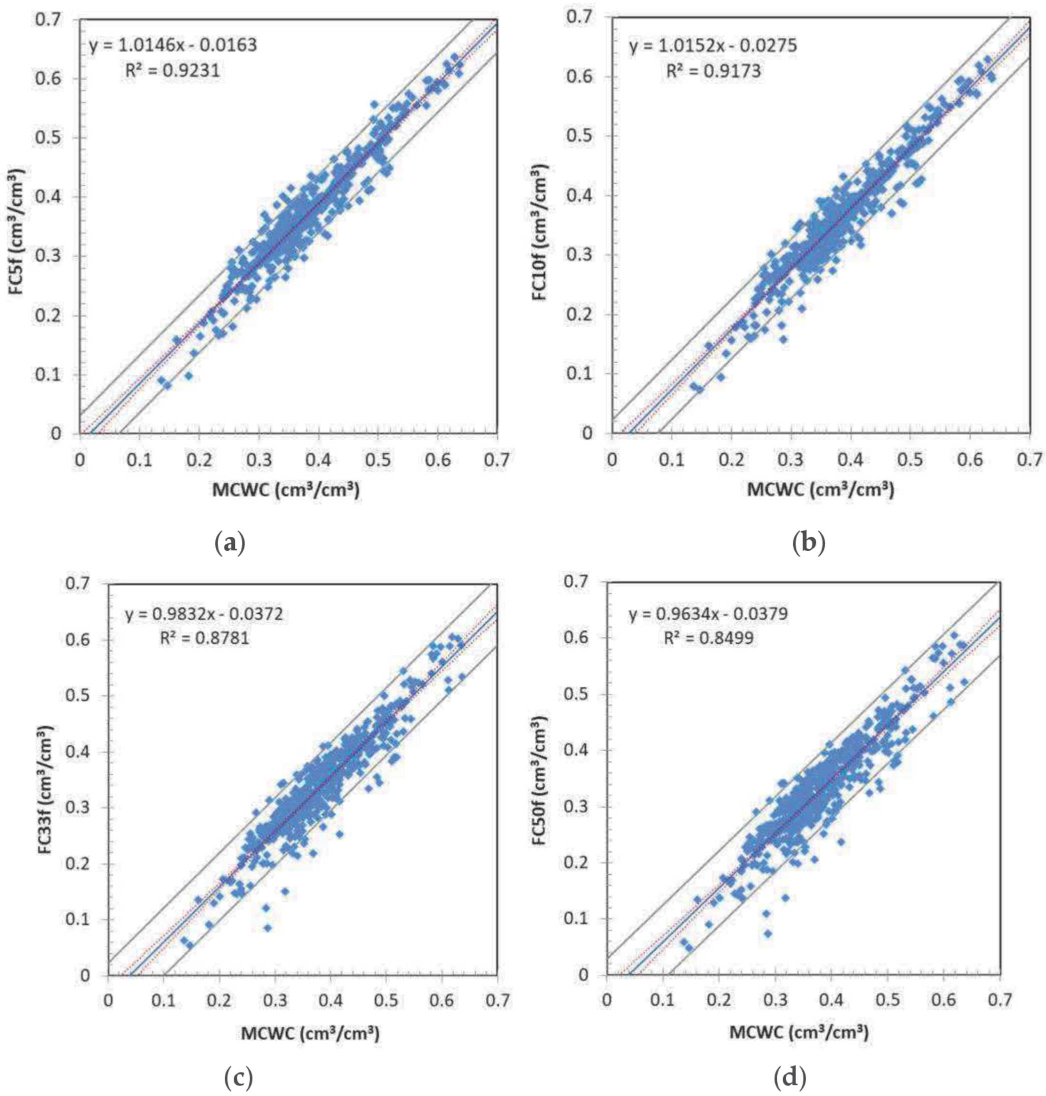


Figure 3. Measured soil moisture constant MCWC and fitted FC selected for several suction pressures, including −5 kPa (**a**), −10 kPa (**b**), −33 kPa (**c**) and −50 kPa (**d**). Confidence (red) and prediction (grey) intervals are provided (0.95).

Table 5. Uncertainty analysis of observed and predicted data.

Correlated Soil Moisture Constants		N	RMSE	MAE	R	R^2
MCWC	FC5f	534	0.027	0.020	0.961	0.923
	FC10f	534	0.033	0.026	0.958	0.917
	FC33f	534	0.053	0.045	0.937	0.878
	FC50f	534	0.062	0.052	0.922	0.850
FC33m	RWC	207	0.045	0.041	0.953	0.908
	MCWC	207	0.065	0.060	0.905	0.818
FC33f	FC by Brežný	471	0.065	0.048	0.669	0.447
	FC by Váša	471	0.067	0.050	0.673	0.453

MCWC—maximum capillary water capacity; RWC—retention water capacity; FC—field capacity; 5, 10, 33, 50—suction pressure (kPa, in abs. value); f—fitted; m—measured; N—number of pairs compared; RMSE—root mean squared error; MAE—mean absolute error; R—correlation coefficient; R^2—coefficient of determination.

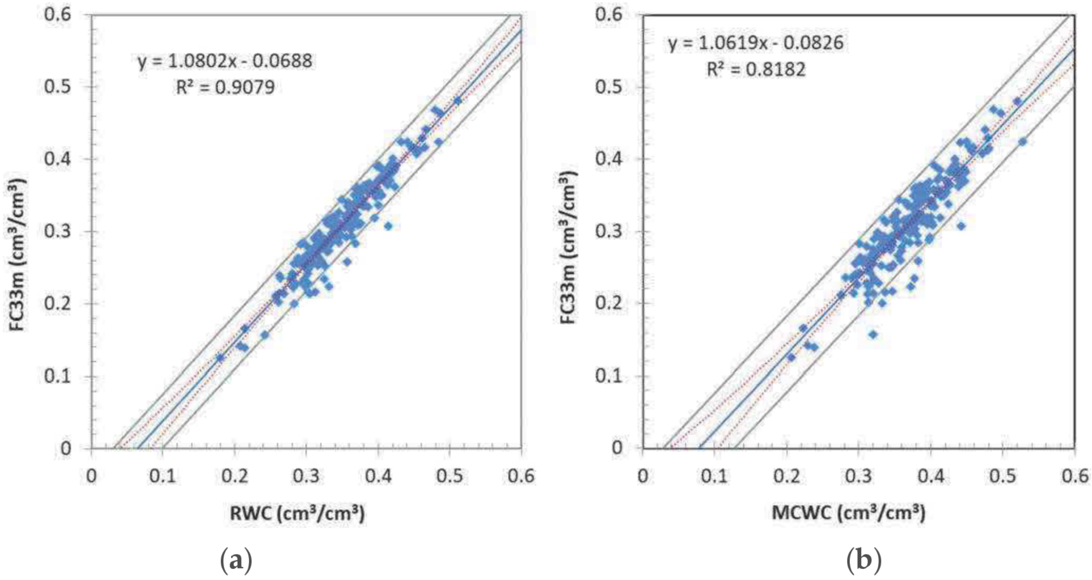
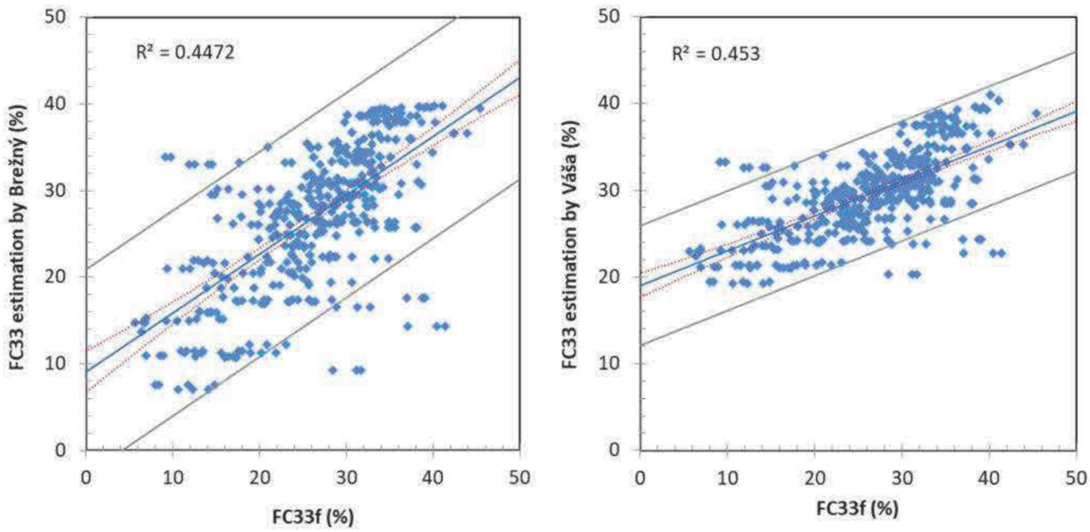


Figure 4. Scatter plots of FC as volumetric water content determined at suction pressure of −33 kPa and soil moisture constants RVC (**a**) and MCWC (**b**). Confidence (red) and prediction (grey) intervals are provided (0.95).

3.3. Results of Testing the Historical Pedotransfer Functions for Field Capacity Estimation

In dataset three, FC33f was estimated from FPSF by employing the equations FC by Brežný (Equation (2)) and FC by Váša (Equation (3)). The uncertainty analysis revealed rather modest correlations, with low R and R^2 values, which is indicative of a moderate linear relationship. Moreover, the RMSE and MAE values are notably higher than those observed in the earlier datasets. This implies a significant level of discrepancy between the observed and predicted values. Ultimately, the performance of these PTFs is shown in Figure 5. The FC by Brežný (Figure 5a) exhibits slightly better performance than the FC by Váša. However, none of them can be recommended for general use. Similarly to FC33f, the estimation of other fitted field capacities, FC5f, FC10f and FC50f, using Equations (2) and (3) was tested as well. However, the results were rather worse; thus, only the FC33f estimation is presented.



(**a**) (**b**)

Figure 5. Testing of relationships of Brežný (**a**) and Váša (**b**) for estimation of field capacity (determined as fitted value calculated using van Genuchten's equation at suction pressure of −33 kPa). Confidence (red) and prediction (grey) intervals are provided (0.95).

4. Discussion

While the present study revealed an increase in both RMSE and MAE between the MCWC and soil water content at gradually increasing suction pressures (in absolute value), it is worth noting that the error magnitudes remained comparatively low. Additionally, a similar trend was observed for the minor decrease in R and R^2 values obtained (see Table 5, Figure 3). As the suction intensifies, water is drained from progressively smaller and potentially more varied pores. The increased suction pressures when considered with soil hysteresis might also reduce the soil's hydraulic connectivity, potentially leading to water entrapment [27]. Despite the slight increase in error and decrease in linearity with rising suction pressures, the relationship between MCWC and water content across the specified suction pressure values can still be considered linear to a significant degree.

MCWC is described [12] as the ability of the soil to retain water for plant needs. The presence and distribution of water within the soil pores continues to be influenced by gravity. The classification of water holding properties according to MCWC, from very poor water retention (MCWC < 5%) to very strong water retention (MCWC > 50%), is presented in Spasić et al. [12]. Good water retention occurs when the MCWC is between 10 and 30%. Compared to MCWC, RWC represents a rather steady state of soil moisture content close to negligible internal drainage. The influence of gravity no longer applies; the water in the pores is under the exclusive influence of capillary forces, specifically in capillary pores. Therefore, this value can represent the quantity of capillary pores in the soil.

The correlation between RWC and FC33m is very strong. This precision and accuracy are evident when evaluated in terms of the relatively short duration of MCWC determination (Table 5, Figure 4). Although MCWC presents a significant correspondence to FC33m given its more rapid assessment period, the disparities between the two measurements may underscore the importance of drainage duration. The FC at −33 kPa inherently represents an equilibrium state between the drained larger pores and the water-retaining smaller-capillary pores, which is better reflected by RWC than by MCWC.

Despite this fact, MCWC remains a more widely used soil moisture constant. MCWCs were extensively obtained during the General Soil Survey of Agricultural Soils (GSSAS), which took place in former Czechoslovakia in the years 1961–1970. Averaged MCWC values for different genetic soil types are presented in the study of Vopravil et al. [14]. The Stagnosols, together with Gleysols, exhibited the highest average MCWC (approx. 41%), while the Luvisols and Leptosols showed the lowest values (approx. 34%), and Cambisols, Fluvisols, Chernozems and Phaeozems were in between with approx. 36–37%. Pospíšilová et al. [28] pointed out that MCWC determines the value of maximum saturation of soil capillary pores. For loamy soils, it should not exceed 36%; otherwise, it shows problems with water infiltration. It is therefore the maximum water content to which the soil should be irrigated without the risk of water losses or waterlogging. Marfo et al. [29] selected MCWC as one the soil properties when assessing the soil's fertility and productivity in their study on ecotone dynamics in the forest–agriculture land transition. They observed a decline in its value in the ecotone area.

Simple linear relationships for the approximation of soil properties are a rather popular form of PTF application. As an example, the linear relationship determined by Němeček et al. [30], which was widely used for the recalculation of clay fractions from a clay fraction of <0.001 mm (%) to a clay fraction of <0.002 mm (%), can be presented. This relationship was applied during conversion between the Taxonomic Classification System of Soils of the Czech Republic and the World Reference Base for Soil Resources [31]. The determination coefficient R^2 of the presented linear regression was 0.9748.

As further examples, historical linear regression equations relating an FPSF to the WP, such as the equations by Váša, Solnář or Brežný [13], can be presented. These equations complement Equations (2) and (3) tested in this study and are still in use, although their reliability is questionable, as demonstrated by the results of this study.

Litschmann et al. [32] introduced a novel approach for the evaluation of moisture and temperature conditions in potato cultivation. In their study, soil moisture was expressed as the % of available water capacity (AWC), which is calculated as the difference between the FC and WP, and should not fall below 60% of AWC when growing potatoes. The equations by Brežný were included for obtaining FC and WP indirectly. Litschmann et al. [33] conducted a comprehensive study on determining FC through the permanent measuring of soil moisture after abundant rainfalls. They employed the equation by Brežný for FC inversely to obtain the value of FPSF, and consequently, used an equation by Brežný for WP calculation, which was 5.4% by volume. The researchers report fairly good agreement inversely with the values previously published for this site. On the national level, the equations by Brežný were used by Novák [34] in the area assessment of dried-up soils in the Czech Republic.

Haberle et al. [20] conducted research onto the associations between the 13C discrimination observed in specific plant species and the spatial heterogeneity of soil properties within agricultural fields. These soil properties were pertinent to the influence of water scarcity on crop productivity. 13C discrimination serves as an indicator of water stress in plants. Their investigation revealed the impact of drought through statistically significant correlations between 13C discrimination during arid periods and soil properties such as AWC. To support their analysis, they derived FC and WP values using the methodology established by Brežný.

Similarly, Haberle et al. [35] used the equations by Váša in their study on the comparison of the calculated and experimentally determined available water supply in the root zone of selected crops.

Vlček and Hybler [19] conducted a rather extensive study to test different simple regression-type PTFs for estimating FC and WP, including the equations by Váša. Among the tested models of PTFs, the equations by Váša showed the poorest performance for both soil moisture constants (R 0.89 and 0.81, respectively). However, the researchers highlighted the fact that minimum input data (only FPSF) were utilized.

5. Conclusions

This study investigated the potential of the so called "filter paper draining method" to be used in the rapid and cost-effective indirect determination of FC. The filter paper draining method is based on draining capillary-saturated soil core samples (typically 100 cm^3 in volume) using filter paper at accurate time intervals. While keeping the experimental settings described in detail in the Section 2, it can be summarized that 2 h of draining results in an MCWC soil moisture constant value, while 24 h of draining results in an RWC soil moisture constant value. Adding the time necessary for capillary saturation (1–3 days) and time for oven drying (1 day), MCWC and RWC as predictors for FC can be obtained within 3 to 5 days. It should be noted that expensive devices' capacity, as seen with the pressure plate apparatus or HYPROP, is limited. The capacity of the filter paper draining method can be increased instantly even with a very low budget. In addition, the method is environmentally friendly with minimum energy requirements compared to, e.g., the pressure plate method.

The results of the present study revealed a very strong correlation between MCWC/ RWC and FC determined as soil water content at a selected suction pressure, which allows for the reasonable use of the following equations for indirect FC determination:

- FC determined as soil water content of −33 kPa can be effectively approximated using the equation:

$$\text{FC33} = 1.0802\ \text{RWC} - 0.0688\ (\text{with RMSE} = 0.045\ \text{cm}^3/\text{cm}^3 \text{ and R} = 0.953).$$

- FC determined as soil water content of −5 or −10 kPa can be effectively approximated, respectively, using the equation:

$$\text{FC5} = 1.0146\ \text{MCWC} - 0.0163\ (\text{with RMSE} = 0.027\ \text{cm}^3/\text{cm}^3 \text{ and R} = 0.961) \text{ or}$$

$$\text{FC10} = 1.0152\ \text{MCWC} - 0.0275\ (\text{with RMSE} = 0.033\ \text{cm}^3/\text{cm}^3 \text{ and R} = 0.958).$$

The results of the present study were verified on more than 700 samples covering the range of arable lands of the Czech Republic and thus can be potentially used in three ways:

1. The use of legacy databases containing MCWC and RWC values together with the equations developed in this study.
2. The fast and effective indirect determination of FC in new studies. The potential use of the equations developed in this study out of the Czech Republic should be verified via traditional FC determination.
3. The development of similar, site-specific equations.

The last contribution of this study is the outcome from the testing of the historical PTFs by Brežný and Váša [13,25], which estimate FC from the fine particle size fraction, on a rather big dataset of 471 entries. Despite modern PTF development, these traditional equations are still in use by many researchers. However, according to the results of the present study, they cannot be recommended for the estimation of FC defined as water content at a certain suction pressure.

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List of Abbreviations

FC	Field capacity (cm^3/cm^3 or %)
FC5f	Field capacity determined at suction pressure of −5 kPa; letter f indicates fitted value (similarly for suction pressures of −10, −33 and −50 kPa) (cm^3/cm^3 or %)
FC33m	Field capacity determined at suction pressure of −33 kPa; letter m indicates measured value (cm^3/cm^3 or %)
FPSF	Fine particle size fraction (soil particles < 0.01 mm) (%)
MCWC	Maximum capillary water capacity (cm^3/cm^3 or %)
PTFs	Pedotransfer functions
RWC	Retention water capacity (cm^3/cm^3 or %)
SWRC	Soil water retention curve
WP	Permanent wilting point (cm^3/cm^3 or %)

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A comparison of measured and estimated saturated hydraulic conductivity of various soils in the Czech Republic

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Abstract: The study aims to indirectly determine the saturated hydraulic conductivity (Ks). The applicability of recently-published pedotransfer functions (PTFs) based on a machine learning approach has been tested, and their performance has been compared with well-known hierarchical PTFs (computer software Rosetta) for 126 soil data sets in the Czech Republic. The quality of estimates has been statistically evaluated in comparison with the measured Ks values; the root mean squared error (RMSE), the mean error (ME) and the coefficient of determination (R^2) were considered. The eight tested models of PTFs were ranked according to the RMSE values. The measured results reflected high Ks variability between and within the study areas, especially for those areas where preferential flow occurred. In most cases, the tested PTFs overestimated the measured Ks values, which is documented by positive ME values. The RMSE values of the Ks estimate ranged on average from 0.5 (coarse-textured soils) to 1.3 (medium to fine-textured soils) for log-transformed Ks in cm/day. Generally, the models based on Random Forest performed better than those based on Boosted Regression Trees. However, the best estimates were obtained by Neural Network analysis PTFs in Rosetta, which scored for four best rankings out of five.

Keywords: soil parameter; soil texture; soil property; prediction; comparative assessment

The saturated hydraulic conductivity of soil (Ks) is one of the most important and most widely-used soil parameters and is commonly applied in a number of different geotechnical, environmental, and water investigations and models (Schaap et al. 2001, Mbonimpa et al. 2002, Araya and Ghezzehei 2019, Tuffour et al. 2019). Ks refers to the ease with which the pores of saturated soil/rock transmit water (United States Department of Agriculture 2022). Ks is reported as one of the most important soil properties during the precipitation, snowmelt, flooding and irrigation events, as it determines the water flow behaviour, infiltration rate, runoff generation and deep drainage (Gamie and De Smedt 2018, Araya and Ghezzehei 2019). Various methods have been developed to determine Ks in the field and the laboratory (Klute 1986). However, for larger areas or heterogeneous areas, an unreasonably high number of replicates need to be carried out in order to account for the spatial variability of Ks. Estimates of Ks by means of pedotransfer functions (PTFs) have been researched widely over the last 30 years. Large databases of basic soil properties (i.e. the European Soil Database (ESDB), the Soil Survey Geographic Database (SSURGO)), together with a range of approaches, including high-performance computing, have been used to obtain reasonable Ks estimates. Bouma (1989) introduced the term pedotransfer function, and Minasny et al. (1999) described PTFs as "translating data we have into what we need". The concept of PTFs was based on easily measured and easily-available soil properties, such as soil texture

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and dry bulk density (BD), which were used as predictors to estimate desirable hydraulic properties (e.g. Ks). More recently, numerous PTFs have been proposed for a variety of purposes. Reviews discussing already published PTFs can be found in the works of Wösten et al. (2001), Pachepsky and Rawls (2004) and Vereecken et al. (2010). These works were mainly aimed at predicting soil water retention parameters. In the review of Zhang and Shaap (2019), a detailed description of the statistical techniques leading to the PTFs development for Ks predictions is presented.

Generally, the first types of PTFs were in the form of tabular values based on the soil texture class (e.g. Wösten et al. 1995) and linear/nonlinear regression equations (e.g. Wösten et al. 1995, Minasny et al. 1999). A more recent approach utilises Neural Network analysis (NN), which relates the basic soil properties (predictors) to the required output data (Ks) by an iterative calibration procedure. This approach has been implemented into the user-friendly Rosetta computer program, in which the models published by Shaap and Leij are utilised (Schaap et al. 1998, Schaap and Leij 2000). The current technical progress of high-performance computing and in hydraulic data collection of large databases has enabled the development of data-driven methods such as machine learning (ML). Araya and Ghezzehei (2019) presented ML-based PTFs for Ks prediction using various types of ML algorithms (K-Nearest Neighbours, Support Vector Regression, Random Forest and Boosted Regression Trees). The availability of large background soil databases implemented into the Rosetta program (Schaap et al. 2001) and ML-based PTFs (Araya and Ghezzehei 2019) made them widely applicable. In this study, the hypothesis that PTFs are robust enough to predict Ks of soils of the Czech Republic with acceptable accuracy is tested.

MATERIAL AND METHODS

Background Ks data. A total of 126 Ks measurements, together with information about soil texture, BD and organic carbon (C_{org}) content, were utilised for this study. The Ks data summarised within the HYPRESCZ database (Miháliková et al. 2013) were enriched by 46 recent own measurements. The data originates from agricultural soils in 13 localities in the Czech Republic (Figure 1). The basic information, together with the relevant soil characteristics, is presented in Table 1. The soil classification is presented in Figure 2. The USDA textural triangle consists of 12 texture classes; however, the FAO textural triangle defines 5 texture classes only. In the Czech Republic, the 12 USDA classes are grouped into 5 "grouped texture classes," according to Němeček et al. (2001), which are similar to the FAO texture classes.

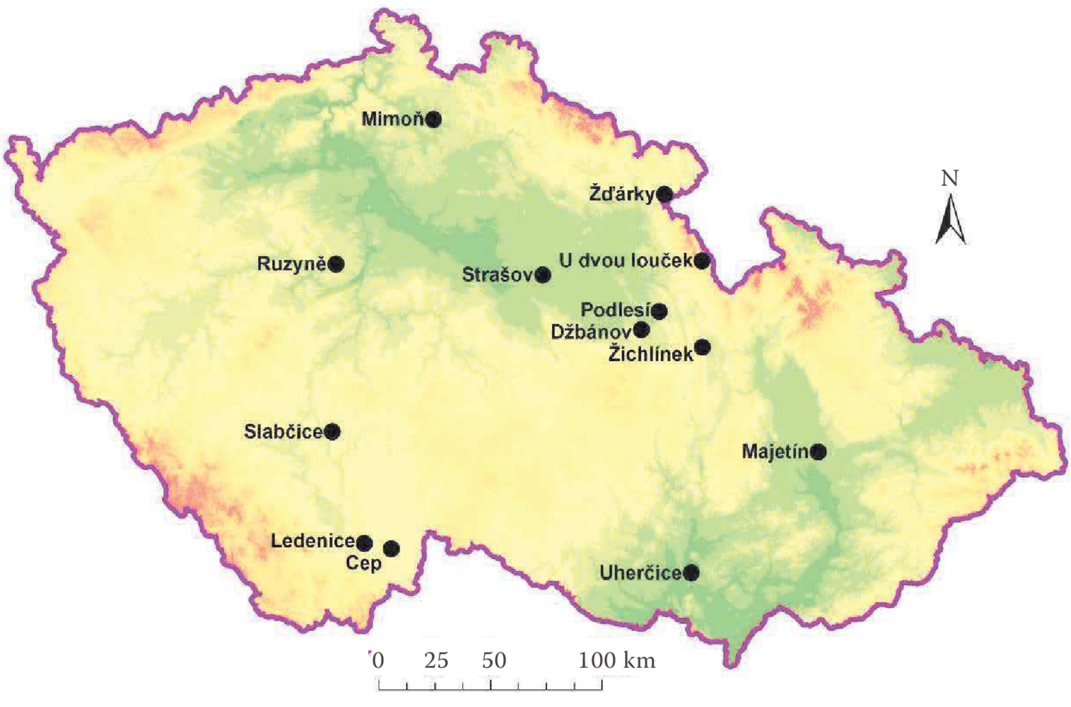

Figure 1. Location of the sites under investigation within the Czech Republic (background map: Czech Office for Surveying, Mapping and Cadastre)

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Table 1. A description of the soils used for pedotransfer function (PTF) application; data for a total of 126 soils are grouped and described in terms of dry bulk density (BD), organic carbon (C_{org}) and saturated hydraulic conductivity (Ks)

USDA texture class	Grouped texture class	Records No.	Averaged BD (g/cm^3)	BD range (g/cm^3)	C_{org} range (%)	Averaged C_{org} (%)	Averaged measured Ks (cm/day)
Sand	1	5	1.41	1.25–1.53	0.46–1.02	0.62	503.29
Loamy sand	1	6	1.34	1.07–1.70	0.27–1.32	0.81	178.18
Sandy loam	2	13	1.47	1.07–1.89	0.17–2.65	1.42	44.09
Loam	3	14	1.57	1.39–1.79	0.06–1.62	0.64	33.13
Silt loam	3	26	1.38	1.01–1.62	0.00–2.90	1.22	245.33
Silt	3	0	na	na	na	na	na
Sandy clay loam	4	15	1.45	1.22–1.73	0.06–3.31	2.34	87.02
Clay loam	4	16	1.55	1.26–1.75	0.06–1.69	0.61	7.42
Silty clay loam	4	23	1.39	1.13–1.74	0.08–1.83	1.02	214.04
Sandy clay	5	0	na	na	na	na	na
Silty clay	5	5	1.27	1.13–1.35	1.72–2.61	1.95	128.43
Clay	5	3	1.29	1.18–1.50	0.41–1.95	1.10	11.71

na – not applicable, as no data for this texture class was available

The Ks data were measured by different laboratory and field methods; the constant head apparatus, the falling head apparatus, pressure ring infiltrometer (Matula and Kozáková 1997) and Hood infiltrometer (Umwelt Geräte Technik, GmbH, Müncheberg, Germany) were employed. The possible effect of the measurement method was not evaluated due to the non-existence of any reference method for Ks determination. The predictors were measured by standard procedures; particle size distribution

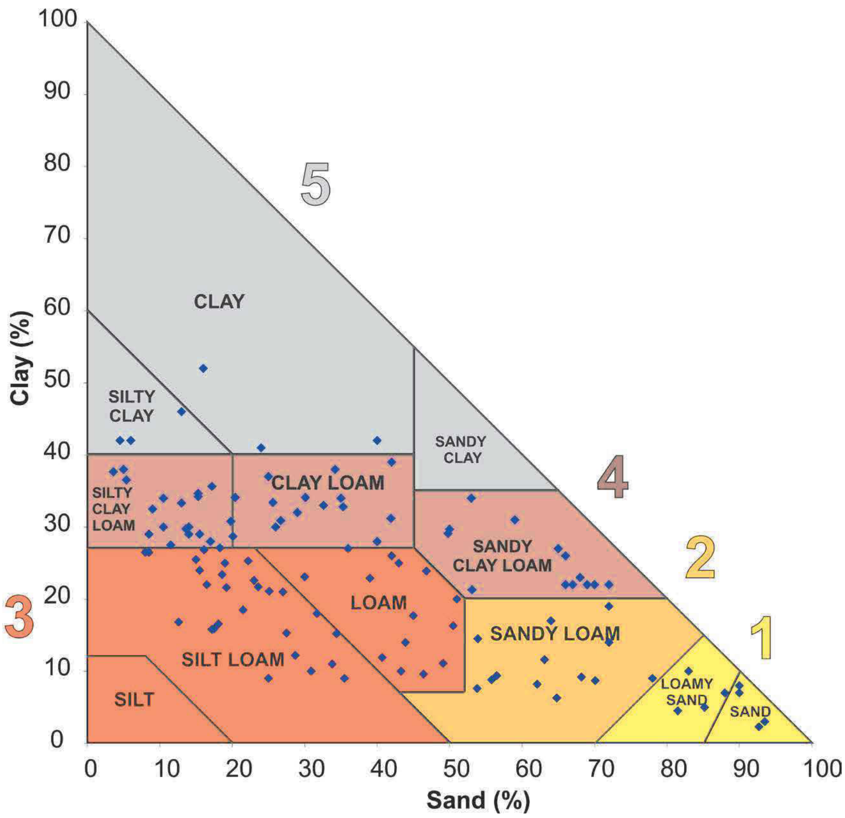

Figure 2. Particle size distribution data of soils used in this study within the USDA soil texture triangle, with coloured indications of the five grouped texture classes (from 1 to 5) according to Němeček et al. (2001)

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analysis by the Hydrometer Method, particle density by the Pycnometer Bottle Method, organic carbon C_{org} by the Walkley and Black oxidometric method, and bulk density on the basis of undisturbed soil core samples (100 cm^3 and/or 250 cm^3).

Applied PTFs. The performance of eight models of PTFs with different predictors was evaluated within this study (Table 2). Aray and Ghezzehei (2019) developed ML-based PTFs on over 18 000 soils based on four types of ML-algorithms, two of which were selected for testing within this study: Random Forest (RF) and Boosted Regression Trees (BRT). The RF method combines (averages) the decisions of the large number of individual decision trees that are "grown" individually by searching for a predictor that ensures the best split that results in the smallest model error. The RF method is reported to be relatively robust to errors and outliers (Gunarathna et al. 2019). BRT provides a form of a decision tree model ensemble with an enhancing procedure by a gradient boosting algorithm that creates additive regression models by sequentially fitting the decision trees (or any different type of "simply based learner") to the current pseudo-residuals at each iteration (Friedman 2002). Thanks to their operating principle, BRT methods are attractive in works where the training data originates from different measurement methods, as in the case of Ks measurements in the field/laboratory when different methods have been applied (Araya and Ghezzehei 2019).

Rosetta (Schaap et al. 2001) is a public domain Windows-based modelling tool for water and solute transport within a variably saturated medium. In total, 1 306 soil samples with a measured Ks value are incorporated within the Rosetta database. It offers five hierarchical PTF models for Ks prediction; two of them were tested in this study (Table 2). Neural Network can be described as a highly interconnected network consisting of many simple processing units that are referred to as neurons (by analogy with the biological neurons in the human brain). Neurons that have similar characteristics are arranged in the NN in groups that are referred to as layers. The neurons in one layer are not mutually connected, but they are connected to the neurons in the adjacent layer. The connection strength of the neurons in the adjacent layers is represented by a parameter referred to as the connection strength or the weight. The NN normally consists of three layers: the input layer, the hidden layer and the output layer (Parasuraman et al. 2006, Arshad et al. 2013).

Statistical evaluation. Ks values expressed in cm/day are presented and evaluated, as it enables comparisons with other published studies. Prior to any statistical evaluation, all Ks values were log-transformed in order to obtain their normal distribution. The performance of the tested PTFs was measured in terms of the root mean squared error (RMSE), the mean error (ME) and the coefficient of determination (R^2), as follows:

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

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

$$R^2 = \left\{\frac{n\sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{\sqrt{[n\sum_{i=1}^{n} x_i{}^2 - (\sum_{i=1}^{n} x_i)^2]\,[n\sum_{i=1}^{n} y_i{}^2 - (\sum_{i=1}^{n} y_i)^2]}}\right\}^2 \quad (3)$$

Table 2. List of applied pedotransfer functions (PTFs) and their predictors

PTF model	Predictor	Reference
BRT 3-0	% sand, % silt, % clay	Araya and Ghezzehei (2019)
BRT 3-1	% sand, % silt, % clay, BD (g/cm^3)	
BRT 3-2	% sand, % silt, % clay, BD (g/cm^3, C_{org} (%)	
RF 3-0	% sand, % silt, % clay	
RF 3-1	% sand, % silt, % clay, BD (g/cm^3)	
RF 3-2	% sand, % silt, % clay, BD (g/cm^3), C_{org} (%)	
Rosetta-SSC	% sand, % silt, % clay	Schaap et al. (2001)
Rosetta-SSC, BD	% sand, % silt, % clay, BD (g/cm^3)	

BRT – Boosted Regression Trees; RF – Random Forest; BD – dry bulk density; C_{org} – organic carbon

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

The RMSE indicates the average deviation of the predicted Ks values from the measured Ks. The smaller the RMSE value is, the better the performance of the PTF prediction. The performance of each PTF model was evaluated according to its rank on a scale from 1 to 8; the best ranking value (1) was attributed to the applied PTF with the smallest RMSE value. The ME is negative if the prediction underestimates the Ks value and is positive if the PTF overestimates the measured Ks. The correspondence between the measured and predicted data is indicated by the R^2 value: the higher the R^2, the better the correspondence.

RESULTS AND DISCUSSION

A total of 126 Ks values were predicted by eight models of PTFs. The soils investigated are rather heterogeneous and involve soils from two to six USDA soil texture classes. Evaluation and ranking of each applied PTF model were carried out in terms of the individual localities and also in terms of the five grouped texture classes (Němeček et al. 2001). The data distributions through their quartiles are graphically displayed in Box and Whisker plots (Figure 3). Generally, a quite high natural variability within and between the localities was observed, especially in the case of agricultural fields, where the tillage operations can temporarily affect the topsoil hydraulic properties. Relatively low variability in measured Ks and relatively good agreement between predicted and observed Ks were found for soils with a coarser texture (Figure 3, texture groups 1 and 2). Relatively high variability in measured Ks was found for soils with medium-to-fine textures (Figure 3, texture groups 3, 4 and 5), where Ks ranged approx. from 0.1 to 1 000 cm/day. For these groups, Rosetta SSC was not able to predict the wide range of measured Ks data (light green).

The quality of the predictions can be observed on the correlation graphs, where predicted and measured Ks data are plotted. The performance of the individual applied models of PTFs for each grouped textural class is displayed in Figure 4, while the comparison for the individual localities is displayed in Figure 5. Stronger correlations can be observed for models using NN analysis and the RF algorithm for coarse-textured soils (texture groups 1 and 2). The

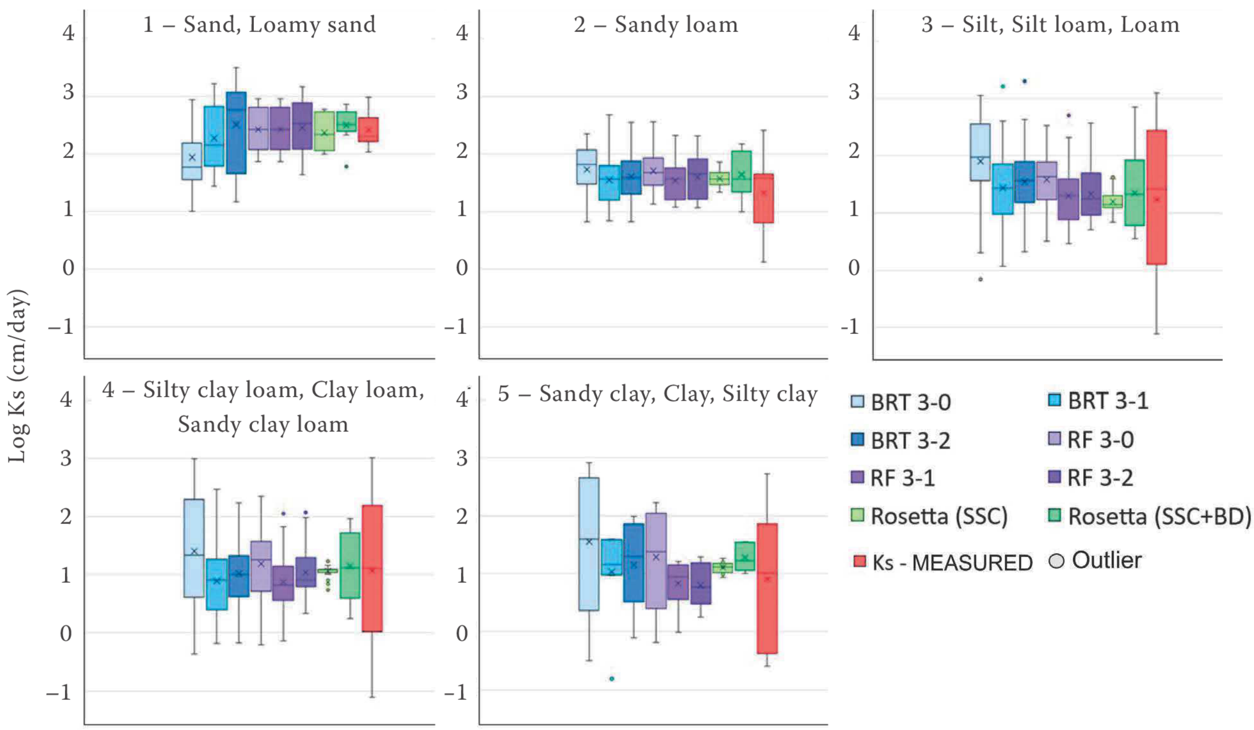

Figure 3. Comparison of the measured (in red colour) and predicted saturated hydraulic conductivity (Ks) values by means of Box and Whisker plots. BRT – Boosted Regression Trees; RF – Random Forest; BD – dry bulk density

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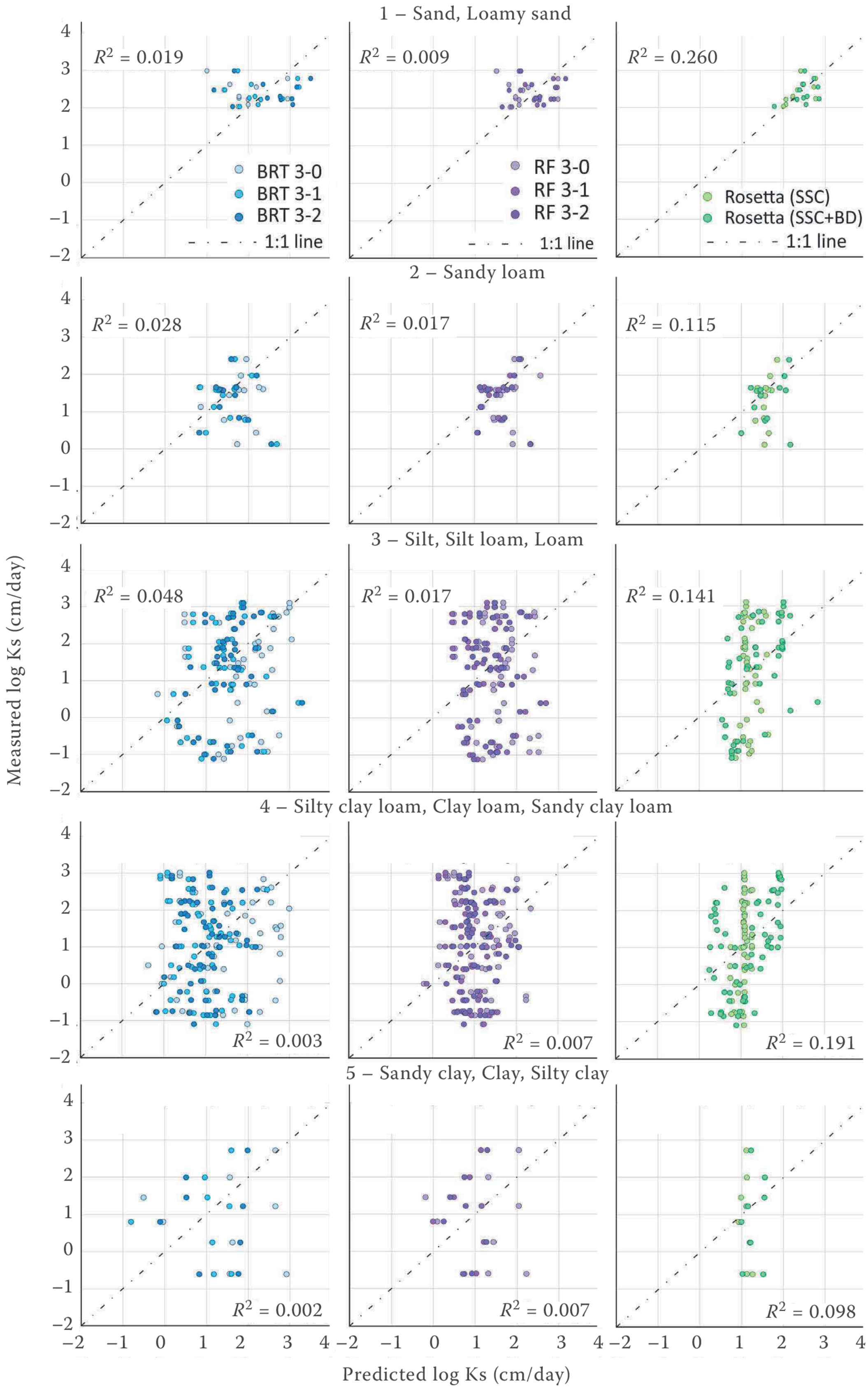

Figure 4. Correlations between the measured and predicted log-transformed Ks data for the soils in the Czech Republic with respect to their attribution to the grouped texture classes (1–5)

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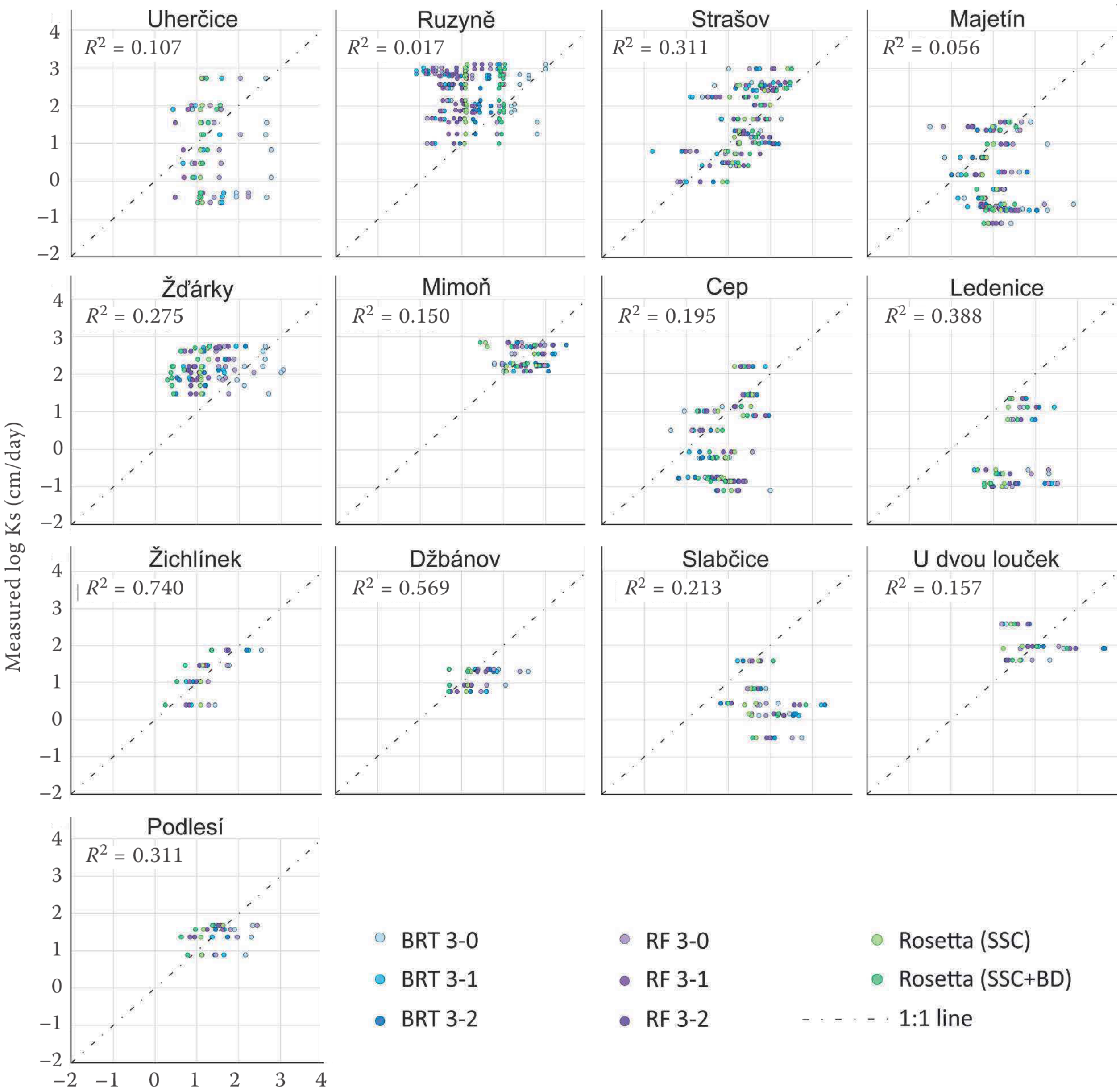

Figure 5. Correlations between the measured and predicted log-transformed saturated hydraulic conductivity (Ks) data for each of the localities in the Czech Republic. BRT – Boosted Regression Trees; RF – Random Forest; BD – dry bulk density

R^2 coefficients ranged from 0.002 (BRT models for texture class 5) to 0.260 (Rosetta models for texture class 1). Very good predictions were observed for the Žichlínek locality (R^2 = 0.740). However, a high R^2 coefficient does not always point to high-quality predictions. This is well illustrated in Figure 5, in the case of the Ledenice locality, where the R^2 coefficient reached a relatively high value of 0.388, but Ks was significantly overestimated in practically all cases. For this reason, the final evaluation and ranking of the applied PTFs were made on the basis of RMSE (Table 3). The best ranking (1) is attributed to the PTF, with the smallest RMSE value summarised for all five grouped texture classes. The effect of overestimation or underestimation of the Ks values is shown in Figure 6, where the ME for each applied PTF and grouped texture class is plotted. Sparse underestimated Ks values originated randomly from all five grouped texture classes; no trends or texture dependency can be observed for the ME values.

In conclusion, the best performance was by the Neural Network models in Rosetta, followed by the

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Table 3. Performance and the final ranking of the tested pedotransfer functions (PTFs) based on root mean squared error (RMSE)

Grouped texture class*	BRT 3-0	BRT 3-1	BRT 3-2	RF 3-0	RF 3-1	RF 3-2	Rosetta (SSC)	Rosetta (SSC + BD)
RMSE values (log Ks in cm/day)								
1 (11)	0.825	0.605	0.783	0.597	0.430	0.493	0.256	0.318
2 (13)	0.841	0.881	0.857	0.745	0.734	0.754	0.621	0.700
3 (40)	1.499	1.367	1.307	1.513	1.418	1.306	1.265	1.122
4 (54)	1.520	1.399	1.306	1.326	1.341	1.240	1.153	1.072
5 (8)	1.791	1.322	1.365	1.493	1.157	1.134	1.168	1.146
Ranking according to RMSE for each Grouped texture class								
1 (11)	8	6	7	5	3	4	1	2
2 (13)	6	8	7	4	3	5	1	2
3 (40)	7	5	4	8	6	3	2	1
4 (54)	8	7	4	5	6	3	2	1
5 (8)	8	5	6	7	3	1	4	2
Sum of rankings**	37	31	28	29	21	16	10	8
Ranking 1–5 (126)	**8**	**7**	**5**	**6**	**4**	**3**	**2**	**1**

*The values in brackets denote the number of soils within each grouped texture class. **The best ranking (1) is attributed to the PTF with the smallest value of the sum of the individual rankings within the grouped texture classes. BRT – Boosted Regression Trees; RF – Random Forest; BD – dry bulk density

Random Forest models, while the ranking of the Boosted Regression Trees models was the poorest. The prediction quality increased with an increasing number of predictors, which corresponds with the findings of Schaap et al. (2001). The Rosetta SSC-BD model, based on the known % content of clay, silt and sand particles, together with information on BD, outperformed all other models (Table 3). However, machine learning techniques have great potential and show promising results (Tóth et al. 2015, Araya and Ghezzehei 2019). The RMSE values for the models using RT reported by Lilly et al. (2008) were on an average 0.97; Tóth et al. (2015) reported an RMSE range from 0.90 to 1.36, while RMSE reported by Araya and Ghezzehei (2019)

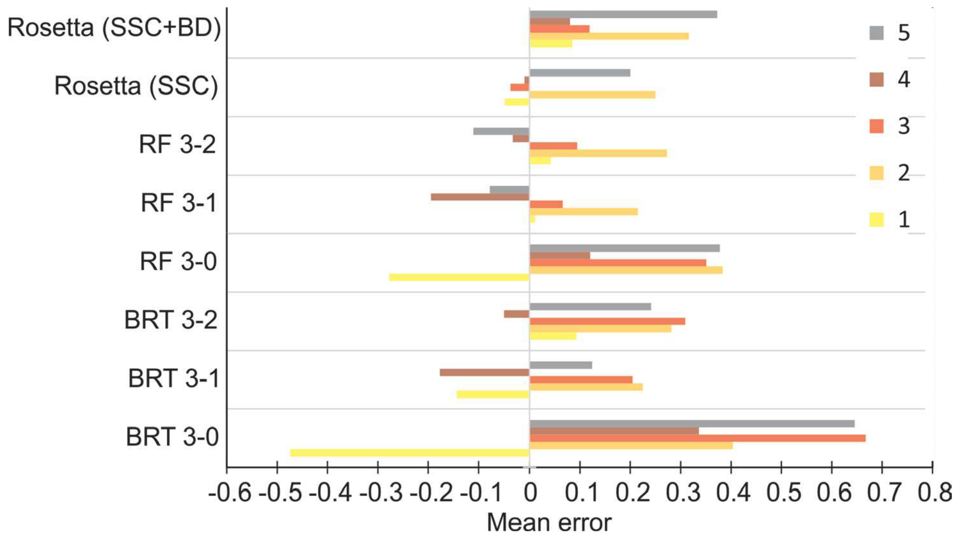

Figure 6. Performance evaluation of the tested pedotransfer functions (PTFs) by means of mean error (ME) for the grouped textural classes (1–5); negative values of ME refer to an underestimation in comparison with the measured values (log Ks in cm/day). BRT – Boosted Regression Trees; RF – Random Forest; BD – dry bulk density

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reached 0.34–0.44 for the BRT models and 0.37–0.44 for RF. In our study, comparable results with RMSE < 1 were obtained by all eight applied models of PTFs only for the grouped soil texture classes 1 and 2 (sand, loamy sand and sandy loam). A possible reason for not scoring higher might be the properties of the soils within the background soil database of PTFs published by Araya and Ghezzehei (2019), which contains mostly soils with a coarse texture; sand, loamy sand, sandy loam, sandy clay loam. In our upcoming work, we therefore plan to involve soil data from this study into the background database and repeat the performance testing of the PTFs.

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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).

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

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

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:

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

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

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

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

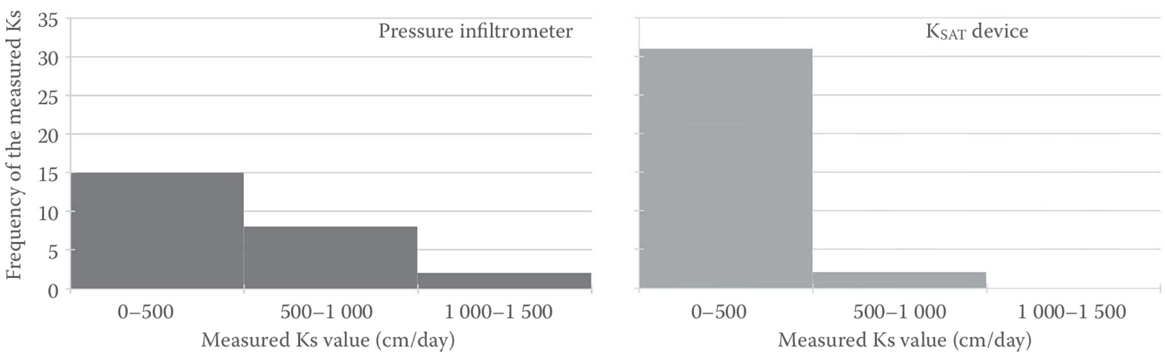

Figure 1. Frequency histograms of the measured saturated hydraulic conductivity (Ks) data; *in-situ* measurements utilising a Pressure infiltrometer by Matula and Kozáková (1997) on the left and laboratory measurements on 250 cm^3 undisturbed soil samples by a K_{SAT} device (METER Group Inc.) on the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

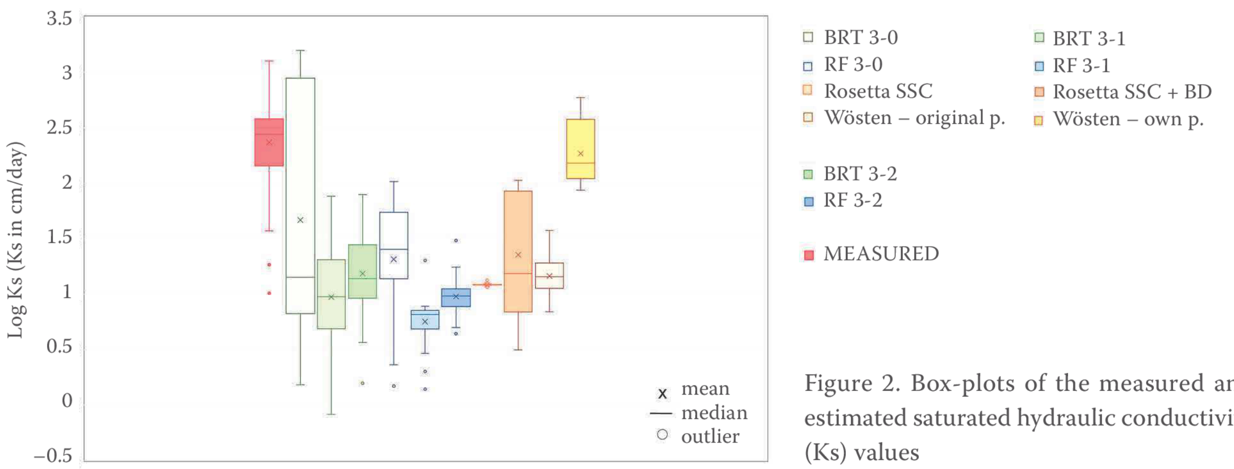

Figure 2. Box-plots of the measured and estimated saturated hydraulic conductivity (Ks) values

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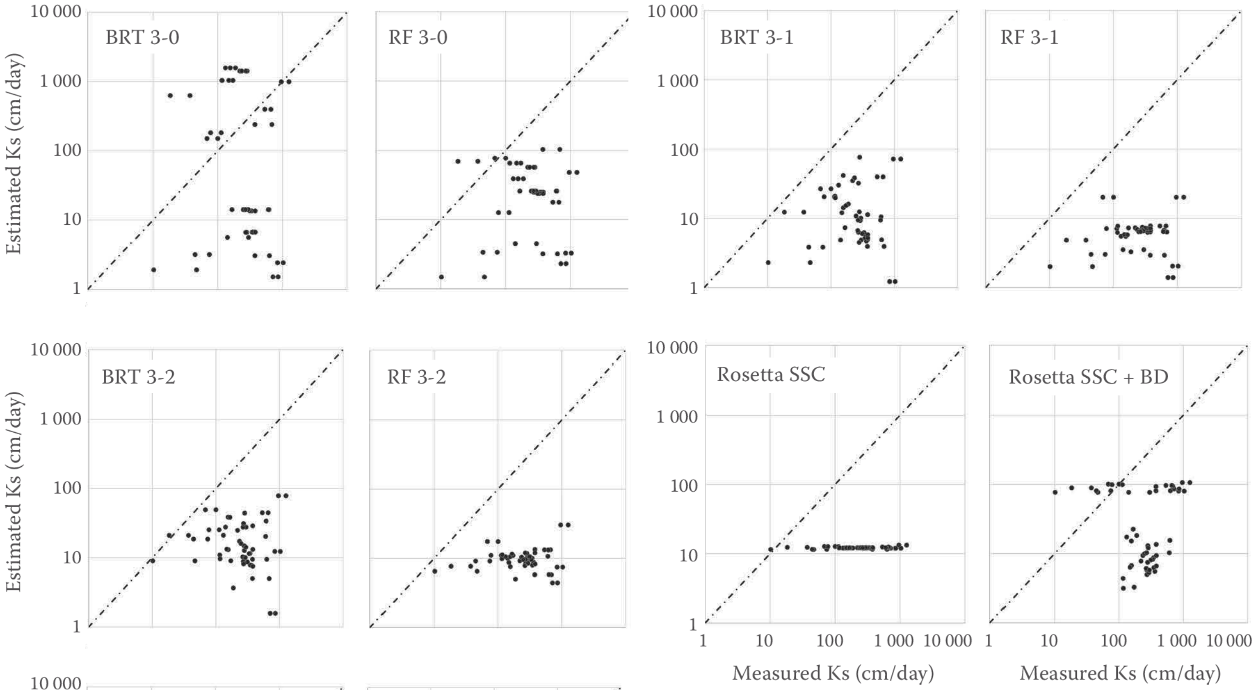

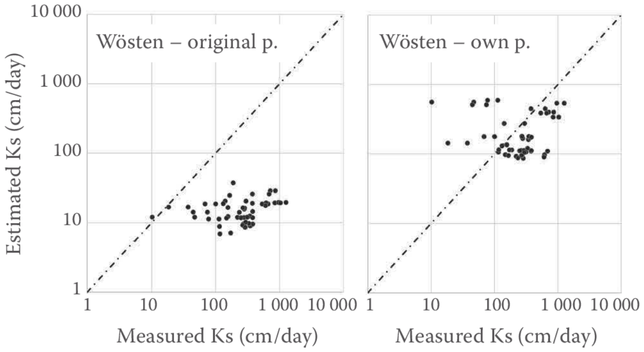

Figure 3. Correlations between the measured and predicted saturated hydraulic conductivity (Ks) data for the individual models of the applied pedotransfer functions (PTFs)

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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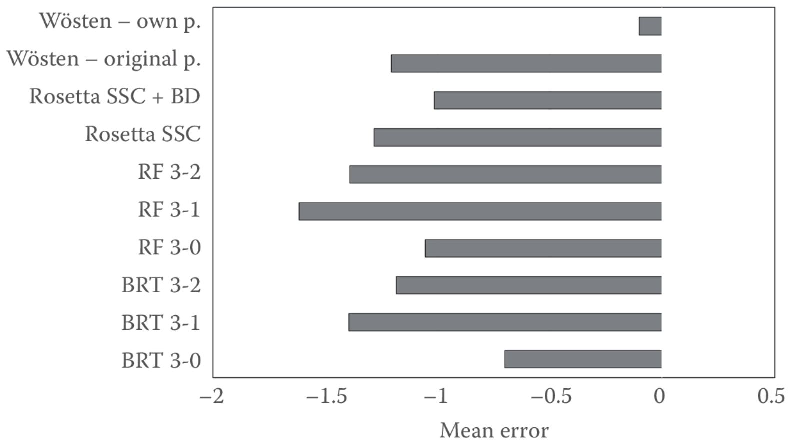

Figure 4. Estimation quality of the tested models of the pedotransfer functions (PTFs) by means of the mean error (ME) The ME values are based on the log-transformed saturated hydraulic conductivity (Ks) values in cm/day

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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4. Summary Discussion

This study series investigates soil hydrophysical properties, organic carbon fractions, surfactant applications, and the estimation of crucial factors such as soil water retention points and Ks. Across the four publications, a cohesive examination unfolds, thoroughly investigating soil properties. The findings yield valuable insights into moisture constants, nutrient dynamics, and hydraulic conductivity, contributing to the ongoing evolution of soil science and water management.

To address the first two objectives, the study of Almaz et al. (2023a) investigated the impact of repeated H2Flo applications on soil properties, revealing a substantial influence on the uniform distribution of soil volumetric water content, particularly at 30 and 50 cm depths. This aligns with established benefits of wetting agents in improving water penetration and redistribution in soils (Oostindie et al., 2008; Dekker et al., 2019). Physicochemical changes included a slight increase in pH (Boomgaard et al., 1987) due to surfactant adsorption, with positive effects observed on electrical conductivity, total organic carbon, and extractable nutrient concentrations (Ogunmokun and Wallach 2021). The shift towards neutral pH enhanced nutrient availability. Changes in nitrogen forms indicated a favourable environment for nitrification. While extractable phosphorus concentrations showed no significant differences, repeated H2Flo applications increased POXC content, highlighting altered degradation conditions, while Cws and Chws contents remained unchanged.

The study identified intricate relationships between organic carbon fractions and nutrient levels, shedding light on the complex interactions induced by H2Flo. Notably, H2Flo applications resulted in a decrease in soil hydraulic conductivity, affecting both Ks and K(h). This decrease in Ks aligns with documented impacts of non-ionic surfactants on sandy soils. Such effects are attributed to factors like soil aggregate disintegration (Mingorance et al., 2007; Liu et al., 2022), pore blockage (Celik et al., 1979; Stellner and Scamehorn 1986), and clay content (Peng et al., 2017). Additionally, the clay content of the soil plays a crucial role in mineral expansion and fine particle mobilization (Peng et al., 2017). These changes tend to occur after multiple applications rather than during the initial application of non-ionic surfactants, which typically results in increased Ks values, especially in hydrophobic soils. Considering the increased POXC and nitrification activity, a potential factor contributing to decreased Ks rates is bioclogging. Research has indicated that bioclogging can lead to a reduction in Ks (Hallett and Young, 1999). When bacteria colonize soils, they form biofilms on pore walls, composed of cells tightly entwined in a network of exopolymer glycocalyx. This coverage reduces the available pore space for water flow, and the exopolymer may also alter soil swelling properties and disperse colloidal particles (Peng et al., 2017). It is noteworthy that some insights are drawn from relatively old studies, as current scientific approaches typically focus on K(h) in experimental designs. The observed decline in Ks values from our study aligns with results from K(h) tests conducted in laboratory settings using soils, both treated and untreated. Similar outcomes have been highlighted in various studies over the past two decades, particularly in non-hydrophobic soils (Mobbs et al., 2012; Bashir et al., 2020). Bashir et al. (2020) specifically associated reduced hydraulic conductivity with slowed vertical movement and increased lateral dispersion of water and surfactant.

Correlations between OCFs and Ks unveil intricate relationships shaped by wetting agents, soil dynamics, and soil organic matter. Existing literature often combines K(h) with dissolved organic carbon (DOC) or particulate organic carbon (POC), leaving a gap in direct comparisons with Ks. Despite this, our data highlights moderate to robust, yet divergent correlations between OCFs and Ks. Water-soluble fractions exhibit a positive association, while POXC shows an inverse relationship with Ks. Notably, although Ks positively correlates with Cws and Chws, it is important to note that treated soils did not exhibit hydrophobic properties in water droplet tests following H2Flo applications.

Almaz et al. (2023a) indicated a progressive decline in Ks rates over time, even in soils without treatment. This trend is primarily attributed to the soil consolidation usually observed throught out the vegetative period (Zhao et al., 2014; Zhu et al., 2022). It is known that changes in Ks are closely linked to alterations in soil structure (Jury and Horton, 2004; Wang et al., 2023) throughout the vegetative cycle, coupled with the effects of emerging decomposition products of organic matter following organic amendments (Dong et al., 2022). These elements collectively impact the soil's capacity to retain water and determine its available water content. The total and readily available water content in soils is typically calculated using the water content at FC and at the WP. Determining the FC and WP is equally crucial as the accurate estimation of Ks rates, a process presenting considerable challenges. This complexity is evident whether the estimation is approached through empirical equations, machine learning models, or linear methodologies, as demonstrated in Batkova et al. (2022) and Báťková et al. (2023). Such accurate estimations are essential for effective water resource management, agricultural planning, and a comprehensive understanding of environmental processes.

The knowledge of both hydraulic conductivity and the water-holding capacities of soils is intrinsically linked to soil fertility, irrigation practices, drainage design, and pollution control strategies, underscoring its importance and complexity in the realm of soil and environmental sciences. In this sense, following a comprehensive analysis of soil hydrology, the decomposition products of organic matter, and the nutritional characteristics of sandy loam soil under commercial farming practices in the study by Almaz et al. (2023a), the subsequent study by Almaz et al. (2023b) aimed to develop a practical and straightforward method for estimating the FC and WP of diverse arable soils across the Czech Republic while providing insights on their hydraulic properties.

To achieve the third objective of the study, the time-consuming aspect of traditional FC and WP determination was addressed by Almaz et al. (2023b). Subsequently, relatively simple RWC and MCWC determinations for various soils were performed, examining their correspondence and linearity with water content at FC under varying suction pressures. Despite observing increased error measures, specifically RMSE and MAE, with rising suction pressures, it is crucial to emphasize that error magnitudes remained remarkably low (e.g., correlation coefficient r varying from 0.905 to 0.961). This consistent low error magnitude indicates a generally linear relationship, particularly at lower suction pressures. The persistence of this linear relationship is noteworthy, especially considering the diminishing influence of gravity on water distribution within soil pores, as elucidated by MCWC, and the increasing impact of capillary forces, represented by RWC. As suction intensifies, water drains from progressively smaller and potentially more varied pores. This intensified suction, coupled with soil hysteresis, may reduce the soil's hydraulic connectivity, potentially leading to water entrapment.

Despite a slight increase in error and a decrease in linearity with rising suction pressures, the relationship between MCWC and water content across specified suction pressure values can still be considered linear to a significant degree. It is essential to recognize MCWC as the soil's capacity to retain water for plant needs, with water distribution within soil pores continuing to be influenced by gravity. The classification of water-holding properties based on MCWC, ranging from very poor water retention (MCWC $< 5\%$) to very strong water retention (MCWC $> 50\%$), provides valuable insights into the soil's capacity (Spasić et al., 2023). Specifically, good water retention occurs when MCWC is between 10 and 30%, a critical range for optimal plant growth.

Comparing MCWC with FC determined at -33 kPa (FC33m), a strong correlation is evident. This precision and accuracy, particularly during a relatively short duration of MCWC determination, underscore the importance of MCWC in representing the soil's moisture-holding capabilities. Despite the significant correspondence between MCWC and FC33m, the study acknowledges disparities between the two measurements, emphasizing the crucial role of drainage duration in soil moisture constants. MCWC, derived from the General Soil Survey of Agricultural Soils (GSSAS) in the former Czechoslovakia between 1961–1970, continues to be widely employed. Averaged MCWC values for different genetic soil types, as presented in the study of Vopravil et al. (2020), highlight variations among soil types. This information is invaluable for understanding the water retention characteristics of different soils, with Stagnosols and Gleysols exhibiting the highest average MCWC, while Luvisols and Leptosols show the lowest values.

The historical use of simple linear regression equations, such as those by Brežný (Brežný, 1970) and Váša (Drbal, 1971), has been extensive. However, the study by Almaz et al. (2023b) raises questions about the reliability of these equations, suggesting the need for further scrutiny in their application. In the broader context of soil property modelling, simple linear relationships, such as the one presented by Němeček et al. (2001) for recalculation of clay fractions, are popular. Historical linear regression equations, including those relating FPSF to FC and WP, as presented by Váša, Solnář, or Brežný (Drbal, 1971), have been widely used but demonstrate questionable reliability. Studies by Litschmann et al. (2016) and Haberle et al. (2014, 2020) further explore innovative approaches for evaluating moisture conditions and the associations between soil properties and crop productivity under varying water conditions. These studies demonstrate the continued relevance of methodologies such as those established by Brežný for deriving FC and WP values.

Due to hydrostatic nature of FC characteristics of soils, which depend on the removal of gravitational water and are influenced by the matric potential of the soil's mineral-organic particles, we were able to establish strong linear relationships. However, the determination of the Ks rate is conducted under hydrodynamic conditions, differing fundamentally from FC characteristics. This distinction presents a significant challenge in estimating Ks rates accurately, as hydrodynamic conditions involve complex interactions of water movement within the soil matrix, influenced by a multitude of factors such as soil texture, structure, and organic matter content. Moreover, this contrast in assessment conditions between FC and Ks further complicates the interpretation and application of soil water data in practical scenarios.

While the hydrostatic principles governing FC are relatively straightforward, the dynamics of water flow under hydrodynamic conditions for Ks estimation involve transient states and non-linear behaviors (Elhakeem et al., 2018). These complexities are exacerbated by environmental variables such as temperature (Ye et al., 2009; Yang et al., 2022), soil compaction (regarding its influence on bulk density) (Pagliai et al., 2004; Capowiez et al., 2021), and root activity (Lipiec and Hatano, 2003; Meurer et al., 2020a), which can significantly change the soil's hydraulic properties over time (Blanchy et al., 2023). Consequently, developing robust models for Ks estimation requires not only a deep understanding of these intricate soil-water interactions but also innovative methodologies that can adapt to the variable and dynamic nature of soils in different agricultural and ecological contexts. In this context, Batkova et al. (2022) employed different PTF models along with machine learning algorithms to estimate Ks using auxiliary soil data and evaluated their performance.

Batkova et al. (2022) focused on predicting Ks through the application of eight PTFs in soils with diverse textures, covering two to six USDA (1951) soil texture classes. The study revealed inherent variability in Ks values, with coarser-textured soils exhibiting lower variability compared to medium-to-fine textured soils, particularly in tilled agricultural fields. Evaluation of the PTF models demonstrated varying performance, with Neural Network (NN) models in Rosetta and Random Forest (RF) models outperforming Boosted Regression Trees (BRT) models.

The study emphasized stronger associations observed for coarse-textured soils, highlighting challenges in predicting Ks for medium-to-fine textured soils. The importance of the number of predictors for enhancing prediction quality was underscored, with the Rosetta SSC-BD model, incorporating information on clay, silt, sand, and bulk density, demonstrating superior performance. While machine learning techniques, especially NN and RF algorithms, show promise in improving predictions, the study acknowledged the need for further refinement. The inclusion of diverse soil data in background databases was identified as a crucial step for enhancing the robustness and applicability of predictive models.

The study illustrated the challenges posed by the natural variability of soils, particularly in agricultural fields subject to tillage operations. Notably, the performance of PTFs varied across different texture classes, with stronger correlations observed for NN models and the RF algorithm in coarse-textured soils. Furthermore, the study delved into the nuanced evaluation of prediction quality, emphasizing the significance of the RMSE over the r^2 coefficient. The

Rosetta SSC-BD model emerged as the top performer, surpassing other models in terms of RMSE across all grouped texture classes. The results also addressed the potential of machine learning techniques, acknowledging their promising results (Tóth et al. 2015, Araya and Ghezzehei, 2019) but cautioning the need for continued investigation and optimization. Comparative analysis with previous studies highlighted the importance of background soil databases (Araya and Ghezzehei, 2019), indicating the intention to incorporate study-specific soil data for future evaluations.

Despite the study by Batkova et al. (2022) relying on the utilization of soil particle size distribution, bulk density, and organic matter content in different models to estimate Ks rates, these routinely measured characteristics are usually in a strong relationship with applied tillage practices (Kreiselmeier et al., 2020; Schlüter et al., 2020). These practices influence soil aeration, porosity, mineral particle movement throughout the soil profile, and organic matter degradation, which consecutively alters the Ks rates even in genetically identical soils. To evaluate the performance of different PTF models along with machine learning algorithms under different tillage practices, the study of Báťková et al. (2023) centered on predicting Ks values in an agricultural field with diverse tillage practices since 1995. Despite minimal variations in particle size distribution data over space and time, the study revealed significant variability in Ks values (Šteakauerová and Mikulec 2009; Schwen et al. 2011). Measured Ks values in the field were notably higher than those obtained in the laboratory, potentially due to disturbances during sampling and transportation. The study evaluated the performance of PTFs based on statistical metrics, ranking them according to RMSE. Notably, the PTFs' model by Wösten et al. (1998) demonstrated the best accuracy, with the lowest RMSE value of 0.521 (log cm day^{-1}). This model, refined based on the Czech soil data, aligns with the importance of utilizing national-scale datasets in refining predictive models. This underscores the crucial role of national-scale datasets, in the development and refinement of PTFs. Báťková et al. (2023) provided a detailed analysis of the predicted Ks values for a single agricultural field with a history of diverse tillage practices. The particle size distribution data, essential predictors for each PTF, were found to be relatively consistent over space and time, highlighting the temporal stability of these soil properties. However, the measured Ks values exhibited a wide range (ranged from 10.2 cm day^{-1} to 1261.2 cm day^{-1}), emphasizing the impact of tillage operations on soil hydraulic properties (Mata et al., 2008; Bonder et al., 2013). One notable observation was the discrepancy between Ks values measured in the laboratory and those obtained in the field. This disparity was attributed to potential disturbances during the sampling and transportation processes, indicating the challenges in accurately capturing in-situ conditions. The study engaged in a thorough evaluation of PTF models, ranking them based on RMSE and scrutinizing their performance using correlation graphs.

An interesting aspect emerged concerning the overestimation of Ks values by certain PTF models, notably the BRT 3-0 model. The study attributed these overestimations to slight differences in particle size distribution, underscoring the sensitivity of these models to small variations in input parameters. However, despite such cases of overestimation, the general trend across all tested PTF models was an underestimation of measured Ks values. The correlation coefficients (r and r^2) between measured and predicted Ks values were observed to be low, but the study wisely emphasized that the RMSE should be considered the most suitable characteristic for evaluating Ks estimation quality.

Comparative analysis with other studies, such as those by Lilly et al. (2008), Tóth et al. (2015), and Araya and Ghezzehei (2019), provided valuable context for understanding the performance of the tested PTF models. The discussion also outlined future research directions, emphasizing the planned incorporation of local soil data into machine learning-based PTFs, which is expected to enhance estimation quality. Additionally, the exploration of other parameters reflecting changes in soil properties caused by agrotechnical operations, such as aggregate stability, is highlighted as a prospective avenue for further investigation.

5. Conclusions

The serie of publications provides insights into soil hydrophysical properties, organic matter degradation products, and predictive modelling. The serie begins with a detailed focus on subsurface drip irrigated loamy sandy soil under commercial farming practices, receiving continuous mineral and organic fertilizer inputs. A part of the related field was treated with repeated applications of H2Flo surfactant, which enhanced water distribution but reduced hydraulic conductivity, impacting various soil properties including nutrient availability. Moreover, the increased NO_3^--N/NH_4^+-N ratios and positive correlations between POXC and NO_3^--N, along with negative correlations with NH_4^+-N, suggest accelerated decomposition and increased nitrification under surfactant applications. This observed acceleration in decomposition and increased nitrification aligns with the initial hypothesis of the study, confirming the anticipated influence of surfactant applications on soil properties and nutrient dynamics. The temporal decline in Ks rates of both control and treated soils may result from both the expected soil consolidation throughout the vegetative period and the increased active carbon pool following the organic input. These results reflect the successful achievement of the first and second objectives of this study: to analyze the impact of repeated H2Flo applications on soil properties, including hydraulic conductivity and organic carbon fractions.

In arable soils, the information on Ks rates should be evaluated with the water holding abilities of soils, usually focusing on the total available water content derived from FC and WP of the soils. FC is an attribute of hydrostatic conditions, contrary to Ks rates, and is deeply connected with soils' porosity and matric potential, dependent on the water holding abilities of mineral and organic fractions in soils. In this context, Almaz et al. (2023b) focuses on developing a practical method for estimating FC in diverse Czech soils. It simplifies traditional determinations by examining RWC and MCWC for various soils under different suction pressures and introduces a cost-effective method for estimating FC through strong correlations between moisture constants and FC, with practical applications in legacy databases. However, traditional PTFs for FC estimation from fine particle size fractions are considered unreliable. This fulfillis the third objective of the study: to introduce a novel approach to estimate FC by utilizing moisture constants (Retention Water Capacity and Maximum Capillary Water Capacity) and appropriate statistical models.

Albeit having highly correspondent predictions of FC, it should be noted that Ks is a complex attribute of soils in a hydrodynamic state, usually necessitating in-situ measurements for accurate results. Producing reliable estimations of Ks with auxiliary data based on particle size distribution, dry bulk density, and organic matter content poses several challenges due to its inherent relationship, particularly with pore continuity. Ongoing efforts are merging the mentioned auxiliary data with different PTF models and machine learning algorithms. Therefore, Batkova et al. (2022) and Báťková et al. (2023) focused on machine learning-based PTFs for predicting Ks in Czech Republic soils. However, the machine learning algorithms are not always superior over the traditional regression PTFs. This approach aligns with the second and third hypotheses of the study, indicating that the utilization of appropriate PTFs to estimate soil hydraulic properties, including FC and Ks, can significantly reduce errors and enhance accuracy of estimates. Additionally, considering regional variations in soil characteristics when developing and applying PTFs, resulted in more accurate estimations. The studies by Batkova et al. (2022) and Báťková et al. (2023) align with the last objective of the study, demonstrating that, despite challenges, the integration of additional data with machine learning-based PTF models holds the potential for enhanced accuracy in predicting Ks. Emphasizing the limitations of PTFs in capturing temporal variability, especially induced by tillage operations, underscores the importance of local databases for refining predictions, contributing to the fulfillment of the objectives of this study.

In conclusion, these findings collectively advance our understanding of soil dynamics, urging a nuanced approach that combines both estimated and directly determined values for comprehensive insight into soil properties and their responses to environmental changes. It is crucial to update the national soil property databases over time to monitor changes in soil properties effectively and obtain necessary comparable data to combat land degradation.

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