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### Research papers

# Estimating the soil water retention curve by the HYPROP-WP4C system, HYPROP-based $PC_{NN}$ -PTF and inverse modeling using HYDRUS-1D

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#### ARTICLE INFO

#### ABSTRACT

This manuscript was handled by Corrado Corradini, Editor-in-Chief, with the assistance of Simone Di Prima, Associate Editor

Keywords: Evaporation experiment Deficit irrigation Machine learning Due to the difficulty of direct field measurement, soil hydraulic properties are often obtained in laboratory settings using small undisturbed soil samples or estimated indirectly through pedotransfer functions (PTFs). The pseudo-continuous pedotransfer function ( $PC_{NN}$ -PTF) is a neural network-based approach for estimating soil hydraulic properties. The main objective of this study was to use field soil moisture and tension data to assess soil water retention curves obtained from the HYPROP-WP4C system and the HYPROP-based PC<sub>NN</sub>-PTF. The in-situ soil water retention data were simultaneously acquired using Acclima TDT and MeterGroup MPS-6 sensors (every 30 min, May to September 2020) from 11 hybrid bermudagrass plots under different irrigation treatments in Riverside, California. We utilized extended evaporation and dewpoint methods using HYPROP-WP4C (Meter Group Inc., USA) devices to obtain lab-measured SWRCs. In addition, SWRCs were estimated from Rosetta (Schaap et al., 2001) and by inverse modeling in HYDRUS-1D utilizing in-situ moisture retention data. Although the hysteresis impacted field data, overall, there was a good agreement between the in-situ and lab water retention data for most samples, especially within the pF range of 2–3.5. The PC<sub>NN</sub>-PTF outperformed Rosetta in estimating laboratory (RMSE=0.034 cm<sup>3</sup> cm<sup>-3</sup> vs 0.063 cm<sup>3</sup> cm<sup>-3</sup>) and in-situ soil moisture data (RMSE=0.048  $cm^3 cm^{-3}$  vs 0.082 cm<sup>3</sup> cm<sup>-3</sup>). Inverse modeling of in-situ data also performed well in estimating the SWRC (RMSE=0.043 cm<sup>3</sup> cm<sup>-3</sup>); however, further attention is required in dry and saturated soil conditions. We developed a simple, free, and easy-to-access tool called PC-PTF for estimating the SWRC using the  $PC_{NN}$ -PTF model evaluated in this study. The PC-PTF can be accessed from the Verdi Water Management Group website: htt p://www.ucrwater.com/software-and-tools.html.

#### 1. Introduction

Direct field measurement of soil hydraulic properties poses significant challenges. As a result, these properties are often obtained in the laboratory using small, undisturbed soil samples or indirectly estimated through pedotransfer functions (PTFs) based on the readily available basic properties of the soil. Equilibrium methods, such as pressure plate extractors and sandbox apparatus, are traditionally employed in the laboratory to acquire water retention data. These methods involve establishing hydrostatic equilibrium between a soil sample and a porous medium at a certain pressure head.

The HYPROP system (Hydraulic Property Analyzer, Meter Group Inc., Pullman, WA, USA) is an automated evaporation-based benchtop laboratory system (Schindler et al., 2010b, 2010a) that is increasingly becoming the standard approach for measuring soil hydraulic properties in the laboratory (Haghverdi et al., 2018; Schindler et al., 2016). It has several advantages over traditional equilibrium methods, such as pressure plate extractors and sandbox apparatus, including the rapid measurement of high-resolution soil water retention and hydraulic conductivity data in wet and intermediate ranges, with minimal variability between replicates (Schelle et al., 2013b). The HYPROP measurements can be complemented with dry-end data from the WP4C Dew Point PotentioMeter instrument (METER Group, Inc., Pullman, WA, USA) to capture the entire soil water retention curve (SWRC).

The parametric and pseudo-continuous PTFs (PC-PTFs) can be used to estimate the SWRC (Haghverdi et al., 2012; Patil and Singh, 2016; Singh et al., 2020). The PC-PTF is a strategy for developing PTFs for continuous soil water retention estimation, employing machine learning approaches like artificial neural networks (PC<sub>NN</sub>-PTF) and support vector machines (Haghverdi et al., 2014). This approach learns the shape of the SWRC directly from the actual measured water retention data, making high-resolution measured data crucial for adequate model

https://doi.org/10.1016/j.jhydrol.2024.131657

Received 23 January 2024; Received in revised form 15 May 2024; Accepted 28 June 2024 Available online 14 July 2024

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training (Haghverdi et al., 2018). Haghverdi et al. (2018) developed the first HYPROP-based water retention  $PC_{NN}$ -PTFs models using a Turkish data set and reported promising results. Then, the first international evaporation/HYPROP-based water retention and hydraulic conductivity  $PC_{NN}$ -PTFs were developed by Singh et al. (2021, 2020), utilizing the international dataset published by Schindler and Müller (2017). The outstanding performance of these PTFs (RMSE of water retention = 0.043 cm<sup>-3</sup>, RMSE of hydraulic conductivity (Log K(h)) = 0.52) positions them among the most accurate international PTFs available for estimating soil hydraulic properties.

The reliability of PTFs developed using laboratory data should be examined when applied to new soils outside their training bounds and under field conditions. Laboratory measurements using small soil samples may not accurately represent actual field conditions due to scale mismatch and field variability (Hopmans et al., 2002). While some studies have compared in-situ to laboratory-measured SWRCs (e.g., Campbell et al., 2018; Ishimwe et al., 2018) and evaluated laboratorybased PTFs against field data (e.g., Wassar et al., 2016, and Gribb et al., 2009), there is a notable gap in research comparing HYPROP-WP4C data and HYPROP-based PTFs with in-situ soil water retention measurements.

Inverse modeling (IM) serves as an alternative method for estimating hydraulic model parameters using in situ data collected through transient water flow experiments (Hopmans et al., 2002; Šimůnek et al., 1998a, 1998b). IM allows for the simultaneous estimation of water retention and hydraulic conductivity functions, eliminating the need for achieving hydrostatic equilibrium (Hopmans et al., 2002; Šimůnek et al., 1998a, 1998b). Inverse methods operate by minimizing an objective function that gauges the deviations between measured and predicted variables, such as water retention data. Several studies have utilized the IM technique to estimate hydraulic parameters with the HYDRUS model (da Silva et al., 2020; Ket et al., 2018; le Bourgeois et al., 2016; Naseri et al., 2022; Pinheiro et al., 2019; Rashid et al., 2015; Šimůnek et al., 1999). To achieve a unique solution, input data with a broad range of water content, soil pressure head, and additional retention curve data obtained through simultaneous measurement of pressure head and water content in the soil profile is necessary (Simunek et al., 1999). Recent advancements in soil sensing technologies offer scientists a tool for rapid and accurate measurement of water content and tension. Wang et al. (1998) employed simultaneous measurements of soil water content and tension from TDR probes and tensiometers, respectively, to develop and test infiltration models through IM. Schelle et al. (2013a) proposed that instrumentation of weighable lysimeters equipped with soil moisture and tension sensors can significantly enhance parameter estimation through the inverse solution. In their IM experiments, Rezaei et al. (2016) utilized tension disc infiltration measurements along with TDRderived soil moisture content to compare in-situ and laboratory soil hydraulic properties. However, with some exceptions, there is a shortage of IM studies employing simultaneous in-situ measurements of soil tension and water content for estimating the SWRC.

The main objective of this study was to assess soil water retention data obtained from the HYPROP-WP4C system and the HYPROP-based  $PC_{NN}$ -PTF approach, utilizing in situ soil moisture sensor measurements from irrigated turfgrass research plots in inland southern California. Additional objectives included (I) evaluating the performance of HYPROP-based  $PC_{NN}$ -PTFs against the Rosetta model (Schaap et al., 2001), one of the most widely used parametric PTFs, and (II) comparing the parametrization of the van Genuchten model (van Genuchten, 1980) using HYPROP-WP4C data with those calculated by IM using the HYDRUS-1D model and in-situ soil moisture and tension data.

#### 2. Material and methods

#### 2.1. Study area and irrigation trial

The study site was located at the University of California Riverside

Agricultural Experiment Station  $(33\circ57'47.0''N 117\circ20'13.4''W)$  in Riverside, California, with a well-drained low-runoff Hanford coarse sandy loam soil (websoilsurvey.sc.egov.usda.gov). The study area consisted of 12 hybrid bermudagrass irrigation research plots ( $3.7 \text{ m} \times 3.7$ m), each receiving a different irrigation treatment via a Weathermatic Smartline 4800 controller (Telsco Industries, Inc., Garland, TX, USA). Irrigation levels varied from 39 % to 66 % reference evapotranspiration (ET<sub>0</sub>). Irrigation frequency for half the plots was set to 3 days per week, while the remaining plots were under an "on-demand" irrigation scenario where the smart controller autonomously regulated the frequency based on the evaporative demand. The soil characteristics of the research plots are shown in Table 1. One plot was excluded from this study due to sensor malfunction issues. Readers are referred to (Haghverdi et al., 2021) for more information about the irrigation trial.

#### 2.2. In situ measurements

Near-surface soil moisture data were collected from all 11 plots between May and September 2019. Each plot was instrumented with a pair of SDI-12 Digital Time Domain Transmissometer (TDT) soil water content (Acclima Inc., Meridian, ID, USA) and MPS6 (METER Group, Inc., Pullman, WA, USA) soil tension sensors placed side-by-side at approximately 10 cm of depth. The DataSnap (Acclima Inc., Meridian, ID, USA) and EM50 (METER Group, Inc., Pullman, WA, USA) loggers were used to collect soil moisture data every 30 min. The TDT sensor has a measurement range of 0 to 100 % volumetric water content (VWC) with a 0.06 % resolution and accuracy of  $\pm$  2 %. The MPS6 sensor has a measurement range of 9 to 100,000 kPa with a 0.1 kPa resolution and accuracy of  $\pm$  (10 % of reading + 2 kPa) from 9 to 100 kPa, according to the manufacturer. The MPS6 determines the water potential of its porous ceramic disc, which comes into hydraulic equilibrium with its surrounding soil. The raw data were filtered for obvious measurement errors outside the physically possible ranges. If either of the two measurements (i.e., soil moisture tension and TDT readings) did not contain meaningful readings, data corresponding to that timestamp was disregarded.

Two soil cores (250 cm<sup>3</sup> stainless-steel cylinders – inside diameter: 8 cm, height: 5 cm) from each plot were collected from areas surrounding the soil moisture sensors in early 2020. Initially, all the plots were irrigated to refill the shallow layer to saturation. Soil coring started after a few days when the plots reached their field capacity, with two plots sampled weekly. Sampling continued for approximately one month. Soil moisture sensor readings from all plots were recorded just before soil sampling to develop site-specific linear calibration equations, assuming no sensor-to-sensor variability. No irrigation was applied during the sampling period, leading to a gradual decline in soil moisture due to transpiration and deep percolation. The composite dataset was assumed to represent the wet-to-dry SWRC.

For the TDT sensors, the factory-calibrated raw measurements (*VWC*<sub>sensor</sub>) were plotted against the measured volumetric water content

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ET based Irrigation treatment (%)	Irrigation frequency (days/week)	Clay (%)	Sand (%)	Silt (%)	BD (g/ cm <sup>3</sup> )
39	3	6	24	70	1.81
39	7	4	21	75	1.73
44	3	6	27	67	1.73
44	7	7	39	54	1.74
49	3	7	32	61	1.74
49	7	9	37	54	1.74
56	3	8	32	60	1.65
62	3	8	22	70	1.9
62	7	2	38	60	1.63
66	3	4	31	65	1.62
66	7	9	38	53	1.82

$$VWC_{calibrated} = 0.6909 \times VWC_{sensor} + 0.0568; R^2 = 0.69$$
(1)

For the MPS6 sensors, the measured volumetric water content data were converted to equivalent soil tension values using the VG equation with parameters obtained from HYPROP measurements. Then, the MPS6 soil tension data (*Tension<sub>sensor</sub>*) were plotted against the back-calculated soil tension (*Tension<sub>calibrated</sub>*) values to develop the following linear calibration equation.

$$Tension_{calibrated} = 0.8667 \times Tension_{sensor} + 11.706; R^2 = 0.92$$
(2)

#### 2.3. Laboratory measurements

The laboratory SWRCs were determined for the soil cores using the HYPROP-WP4C system. All samples were saturated. Subsequently, two vertically aligned tensiometers were installed in two holes created with a small auger, positioning the tips of the tensiometers 1.25 cm below and above the center of the cylinder (2.5 cm). Throughout the HYPROP measurement campaigns, the soil tensions at the two tensiometers were automatically monitored using HYPROP-VIEW software, while the weight of each sample was continuously recorded. The measurement campaign spanned 5 to 7 days for each soil sample. Following the completion of HYPROP measurements, the WP4C was employed to measure dry-end (~pF>4) soil water retention data. A total of 4-5 subsamples (each  $\sim 7 \text{ cm}^3$ ) were collected from the top, middle, and bottom of the original undisturbed sample with varying water contents. These subsamples were sliced off the original sample and stored in capped small sample cups (15 cm<sup>3</sup> capacity). The soil tension of each subsample was measured using the WP4C, and the weight of the sample was immediately recorded. Finally, oven-dry weight was obtained for the subsamples and the remaining soil material from HYPROP, which was used to determine the dry bulk density (BD) of the soil (Blake and Hartge, 2018).

The soil hydraulic parameters obtained by fitting the VG model (Eq. (3)) for each soil sample during the evaporation experiment were inputted from the HYPROP-FIT software. HYPROP-FIT works based on a revised version of SHYPFIT2.0 (Peters and Wolfgang, 2015) to estimate the best parameter combination.

$$\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{\left[1 + \left(\alpha h\right)^n\right]^m} \tag{3}$$

$$m = 1 - 1/n \tag{4}$$

where  $\theta$  is volumetric moisture content [cm<sup>3</sup> cm<sup>-3</sup>] at matric potential *h* [cm];  $\theta_r$  [cm<sup>3</sup> cm<sup>-3</sup>]; and  $\theta_s$  [cm<sup>3</sup> cm<sup>-3</sup>] are residual and saturated moisture contents, respectively;  $\alpha$  [cm<sup>-1</sup>] and *n* are curve-shaped parameters. Large values of *n* result in a steeper curve and lower values of  $\alpha$  indicate a larger air-entry value.

#### 2.4. Pedotransfer functions

The laboratory measured data via the HYPROP-WP4C system and field data collected via soil moisture sensors were used to evaluate the performance of  $PC_{NN}$ -PTF (Singh et al., 2020) and Rosetta (Schaap et al., 2001). Fig. 1 shows the textural distribution of the soil cores collected from the hybrid bermudagrass irrigation plots. The  $PC_{NN}$ -PTF (a three-layer feed-forward perceptron NN model) was trained using a combination of the international dataset published by (Schindler and Müller, 2017) and a Turkish dataset by (Haghverdi et al., 2018). Soil texture (SSC), BD and soil tension were used as inputs to the model, and the output was VWC. The hydraulic properties of the soils in both datasets were measured using the evaporation experiments and the HYPROP system. Readers are referred to (Singh et al., 2020) for more information about the development of the international HYPROP-based  $PC_{NN}$ -PTF used in this study.

SWRC estimations using the parametric model Rosetta were also made with SSC and BD as inputs. Rosetta is an ANN-based PTF that uses a hierarchical approach to suit specific cases of input data available to estimate water retention VG parameters, saturated hydraulic conductivity ( $K_s$ ), and unsaturated hydraulic conductivity. Rosetta was used for estimating the VG parameters of the SWRC utilizing the nonlinear leastsquares optimization program RETC (van Genuchten, 1991):

#### 2.5. Inverse modeling using HYDRUS-1D

In this study, the HYDRUS-1D (Rassam et al., 2018; Šimůnek et al., 1998a, 1998b) model was utilized to estimate the in-situ soil water dynamics at the burial depth of the sensors (10 cm). HYDRUS-1D is a computer program that applies the Richards equation (Richards, 1931) for unsaturated, non-steady flow in the soils.

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[ K(h) \left( \frac{\partial h}{\partial z} + 1 \right) \right]$$
(5)



**Fig. 1.** (a) Soil textural distribution of the soil samples used for development (blue) and validation (red) of the PC<sub>NN</sub>-PTF., (b) lab and in-situ measured SWRCs for the validation soils. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

where *t* is time [T], *z* is the vertical distance [L], *h* is the soil moisture tension [L], and *K* is the hydraulic conductivity [L/T] which is a function of *h*.

Soil water flow simulation using HYDRUS-1D requires knowledge of the hydraulic parameters, head and flow boundaries, atmospheric boundary conditions, and time-dependent inputs. Simulations were performed at a daily timestep to better highlight the changes in soil moisture dynamics due to variations of meteorological conditions such as rainfall and evapotranspiration fluxes. The free/zero-gradient drainage boundary condition is suitable for water flow simulation of unsaturated soil in which the soil domain of interest is not affected by groundwater. Therefore, a free drainage boundary condition was assigned to the bottom of the flow domain, and an atmospheric boundary condition was assigned to the soil surface. The atmospheric boundary condition at the surface was described using ET<sub>o</sub> measurements taken from the nearest California Irrigation Management Information System (CIMIS) station #44, located about 260 m from the site. The time-dependent inputs are the combined irrigation and precipitation rate [LT<sup>-1</sup>] (sum of the values for input into the model), evaporation rate  $[LT^{-1}]$ , and transpiration rate  $[LT^{-1}]$ . The evaporation (E) and transpiration (T) rates must be input as separate values, which was achieved as follows (Belmans et al., 1983):

$$E = ET.e^{-k.LAI} \tag{6}$$

$$T = ET - E \tag{7}$$

where *k* is the extinction coefficient for solar radiation and LAI is the plant's leaf area index  $[L2/L^2(-|-])$ . A *k* value of 0.39 was used for HYDRUS-1D simulations. The LAI of hybrid bermudagrass was reported to be low (around 2), especially in the late summer months (Fontanier and Steinke, 2017). Thus, our study assumed LAI to be 2 from May to September.

The observation nodes were set at 10 cm following the location of the TDT and MPS6 sensors. At the beginning of the simulation in the soil profile domain, the soil moisture was set to the initial observation from TDT sensors. HYDRUS-1D estimates root water uptake via the model proposed by (Feddes et al., 1978), where root water uptake rates are assigned according to the soil tension at the point of interest. The root distribution was assumed to be 1.0 (maximum number of roots possible) between the soil surface and a 10 cm depth and to decrease linearly from 1.0 to 0.0 (no roots) from a 10 cm depth to a 50 cm depth.

Inverse solutions to flow problems can be solved where measured data is used to estimate soil hydraulic parameters. For the inverse modeling utilizing HYDRUS-1D, the objective function was minimized using the Levenberg-Marquardt nonlinear minimization (Marquardt, 1963). For the optimization of the initial VG parameters (Table 2), a

combination of three sets of data, i.e., the water content in daily time steps  $\theta(t)$  from the TDT sensors, soil water tension in daily time steps h(t) from the MPS6 sensors, retention pairs  $\theta(h)$  from simultaneous measurements of TDT and MPS-6 were used. Raw sensor data were averaged to obtain mean daily values. All parameters of the VG equation (Eq. (3)) for the SWRC were optimized. Ks data were obtained from the HYPROP-FIT.

#### 2.6. Performance assessment

To evaluate the performance of the SWRCs estimated by  $PC_{NN}$ -PTF and Rosetta PTF, the root mean square error (*RMSE*, Eq. (8)), mean absolute error (*MAE*, Eq. (9)), mean biased error (*MBE*, Eq. (10)), and correlation coefficient (*R*, Eq. (11)) were calculated:

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (E_i - M_i)^2}$$
(8)

$$MAE = \frac{1}{n} \sum_{i=1}^{n} |E_i - M_i|$$
(9)

$$MBE = \frac{1}{n} \sum_{i=1}^{n} (E_i - M_i)$$
(10)

$$R = \frac{\sum_{i=1}^{n} (E_i - \overline{E}) (M_i - \overline{M})}{\sum_{i=1}^{n} (E_i - \overline{E})^2 \sum_{i=1}^{n} (M_i - \overline{M})^2}$$
(11)

where *E* and *M* are the estimated and measured VWC, respectively;  $\overline{E}$  and  $\overline{M}$  are the mean estimated and measured VWC, respectively, and *n* (*lab* = 1016; *in-situ* = 15787) is the total number of measured water retention points for each model. In addition, the error statistics were separately calculated for the wet (pF $\leq$ 2), intermediate (2 < pF $\leq$ 3), and dry regions (pF>3) of the SWRC.

#### 3. Results and discussion

#### 3.1. Comparing the in-situ and laboratory measurements of the SWRCs

The characteristics of the soil samples collected from the irrigated hybrid bermudagrass plots are shown in Table 1. The texture and water retention data are shown in Fig. 1. Samples belonged to loamy sand (n = 1) and sandy loam (n = 10) soil textures. The BD values ranged from 1.49 to 1.90 g cm<sup>-3</sup> with an average of 1.72 g cm<sup>-3</sup>. The slight variability in soil texture and BD among samples shows that spatial heterogeneity exists even in relatively small areas. The bermudagrass plots were under deficit irrigation treatments, with the highest irrigation

Table 2

Van Genuchten (VG) parameters obtained from H	YPROP-FIT, Rosetta, and Inverse mode	eling (IM) for soil samples	from each irrigation treatment
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Irrigation treatment	Fitted (HYPR	Fitted VG parameters (HYPROP-FIT)							Estimated VG parameters (Rosetta PTF)					Optimized VG parameters (IM, HYDRUS-1D)		
	$\theta_r$	$\theta_{s}$	α	n	Ks	L	$\theta_r$	$\theta_{s}$	α	n	Ks	L	$\theta_r$	$\theta_{s}$	α	n
39–3	0.03	0.30	0.012	1.38	1.10	-2.27	0.03	0.30	0.059	1.36	0.78	0.5	0.06	0.21	0.003	1.29
39–7	0.04	0.33	0.022	1.52	8.76	-0.49	0.03	0.32	0.054	1.53	38.78	0.5	0.00	0.29	0.038	1.11
44–3	0.04	0.32	0.020	1.46	1.81	-2.18	0.03	0.32	0.053	1.36	22.92	0.5	0.07	0.29	0.014	1.20
44–7	0.01	0.33	0.012	1.31	2.69	-0.06	0.03	0.30	0.040	1.30	14.47	0.5	0.00	0.26	0.001	1.30
49–3	0.02	0.32	0.017	1.34	5.92	0.37	0.03	0.31	0.049	1.31	17.12	0.5	0.04	0.27	0.009	1.25
49–7	0.00	0.35	0.016	1.24	14.30	0.08	0.03	0.31	0.037	1.29	12.48	0.5	0.00	0.31	0.004	1.22
56–3	0.01	0.34	0.018	1.29	5.26	-0.48	0.03	0.33	0.037	1.36	22.11	0.5	0.15	0.27	0.005	1.35
62–3	0.00	0.31	0.006	1.27	1.63	-2.48	0.03	0.28	0.059	1.31	11.31	0.5	0.15	0.26	0.011	1.29
62–7	0.03	0.37	0.021	1.34	1.62	-3.11	0.03	0.32	0.045	1.37	35.36	0.5	0.09	0.30	0.016	1.29
66–3	0.00	0.36	0.053	1.26	22.20	-1.75	0.03	0.33	0.046	1.41	36.88	0.5	0.08	0.32	0.032	1.21
66–7	0.00	0.37	0.010	1.25	3.27	-0.96	0.03	0.29	0.045	1.25	8.92	0.5	0.14	0.30	0.010	1.46

 $\theta_r$  (cm<sup>3</sup> cm<sup>-3</sup>): residual moisture content;  $\theta_s$  (cm<sup>3</sup> cm<sup>-3</sup>): saturated moisture content;  $\alpha$  [cm<sup>-1</sup>] and *n* are curve shape parameters; m = 1–1/n; K<sub>s</sub>: saturated hydraulic conductivity (cm d<sup>-1</sup>); L is an empirical parameter.

treatment being 66 %  $ET_o$ . This allowed us to have a high range of the insitu soil moisture tension observed in the field, especially from the lowest deficit irrigation treatments, therefore providing retention data ranging from pF (the logarithmic transformation of soil tension in cm of water) equal to 2 up to roughly 4.2 (permanent wilting point) for most of the plots. The laboratory-obtained SWRCs covered the entire curve range from saturation to air-dry tension, with HYPROP data covering the wet and intermediate ranges and WP4C data covering the dry end.

Fig. 2 depicts a time series of soil moisture and tension data measured in the field at 30-minute intervals. Fig. 3 shows the measured and estimated SWRCs in this study. An abrupt steepening of the slope close to the saturation indicates a distinct air-entry value, the tension at which moisture begins to drain from the soil pores. The lab-obtained SWRCs had a similar shape, indicating comparable air entry and the sudden reduction in soil moisture as tension increased. The MP6 sensors had an upper limit of -9 kPa (pF =  $\sim$ 2), which is the air entry value of the sensor, thus resulting in a lack of in-situ water retention points close to saturation (Campbell et al., 2018). There were only a few moisture retention data points in the wet range for the in-situ data because most of the data were greater than the pF value of 2. For instance, only  $\sim 1.5$ % of retention points were in the wet region for the data collected at the 30-minute interval for 2019, ~70 % of data lies in the intermediate range, and  $\sim 28$  % in the dry region. There were no retention points in the wet region for the daily average of data collected during the summer

#### of 2019.

Previous studies have shown that differences between laboratory and field measurements of soil hydraulic properties are attributed to several factors, including hysteresis and entrapped air (Bordoni et al., 2017; Pirone et al., 2014; Schuh et al., 1988), inadequate representation of large pores in the laboratory (Field et al., 1984), spatial variability, sample disturbance (Field et al., 1984; Ishimwe et al., 2018; Schuh et al., 1988), and sample size-related scale effects (Pachepsky et al., 2001; Schuh et al., 1988). The in-situ SWRCs demonstrated good agreement with the lab SWRCs for most samples, particularly within the pF 2 up to approximately 3.5 range. Beyond this point, a more gradual decline in soil moisture was observed as tension increased. This finding aligns with a study conducted by Campbell et al. (2018) on similar soil textures, where they reported strong agreement between lab and in-situ data for pF ranging from around 2 to 3.7 for sandy loam and loamy sand. Notably, Campbell et al. (2018) also employed HYPROP and MPS6, contributing to the observed similarities between the findings of the two studies. However, our field data exhibited more scatter, primarily because Campbell et al. (2018) only used drying in situ data, excluding wetting data that could reveal distinct patterns and deviations from drving data due to hysteresis. In contrast, livama's in-situ SWRCs showed approximately 10 % smaller VWC than the lab SWRCs (livama, 2016). This difference was attributed to the natural conditions of hysteresis, causing the wetting process to consistently yield smaller



**Fig. 2.** Soil volumetric water content (VWC,  $cm^3 cm^{-3}$ ) and soil tension (pF=logarithm of soil tension in cm) time series as measured by the sensors installed at different plots during 2019 at the 30-minute time step. Shaded regions represent the data used in this study when ET-based irrigation treatments were implemented.



Fig. 3. Comparison of measured soil water retention data in the laboratory and field with estimated SWRCs using PC<sub>NN</sub>-PTF, Rosetta, and inverse modeling via HYDRUS-1D.

moisture values than the drying process for a given soil tension. We did not observe the same pattern in all our plots. This is partly attributed to different instruments and sensors used in the two studies for laboratory and field measurements. Iiyama (2016) utilized the hanging-watercolumn and pressure-plate methods for lab SWRC measurement, employing capacitance-type soil moisture sensors and tensiometers in the field. While tensiometers generally offer high accuracy in the wet range, capacitance-type soil moisture sensors typically exhibit low accuracy (Evett et al., 2012).

Table 2 shows the VG parameters from HYPROP-FIT, Rosetta and IM. Since IM was based on the in-situ soil moisture and tension observations, variations in the values of VG parameters obtained from IM and HYPROP-FIT allowed us to identify the differences between laboratory and in-situ SWRCs. The VG parameters  $\alpha$  and n affect the steepness of the SWRC, where  $\alpha$  relates to the inverse of air-entry value and n indicates the steepness of the slope. The parameter  $\alpha$  ranged from 0.006 to 0.53 with an average of 0.019 for the lab SWRCs and from 0.001 to 0.038 with an average of 0.013 for the in-situ VG parameters obtained through IM. The parameter n ranged from 1.24 to 1.52 with an average of 1.33 for the lab SWRCs and from 1.11 to 1.46 with an average of 1.27 for the in-situ SWRCs. This is also evident in Fig. 3, as the air-entry value is lower, and the steepness of the SWRC is higher for the lab-obtained curves than the in-situ curves.

#### 3.2. Performance of the models

#### 3.2.1. In-situ SWRCs

Table 3 summarizes the performance statistics of the PC<sub>NN</sub>-PTF and Rosetta for laboratory and in-situ water retention measurements. PC<sub>NN</sub>-PTF showed RMSE of 0.048 cm<sup>3</sup> cm<sup>-3</sup> for the in-situ data collected at intervals of 30 min during the year 2019, and MBE of -0.012 cm<sup>3</sup> cm<sup>-3</sup> was observed. SWRCs estimated using parameters obtained from Rosetta performed worse than the PC<sub>NN</sub>-PTF with RMSE=0.082 cm<sup>3</sup> cm<sup>-3</sup>. Rosetta showed a tendency to underestimate VWC, indicated by MBE of -0.079 cm<sup>3</sup> cm<sup>-3</sup> for in-situ data, also evident in Fig. 4. Correlation coefficients (R) of 0.91 and 0.90 were observed for PC<sub>NN</sub>-PTF and Rosetta, respectively. The PC<sub>NN</sub>-PTF performed better than Rosetta in estimating the in-situ SWRCs.

Hysteresis refers to the changes in the SWRC due to wetting and drying of the soil in the field. In-situ soil moisture can also be affected by physical processes such as hysteresis, somewhat evident in 30-min soil moisture data of plots under 62 % ETo-3d wk<sup>-1</sup>, 62 % ETo-on-demand, 66 %  $ET_{o}\mbox{-}3d\ wk^{-1},$  and 66 %  $ET_{o}\mbox{-}on\mbox{-}demand$  irrigation treatments. Hysteresis measurement can be challenging both in the laboratory and field due to the lack of enough data to quantify the wetting and drying cycles. Because of the complexities, only the drying hydraulic path is generally considered in laboratory measurements, although drying and wetting alternate in the field. Numerous efforts continue to address the effects of hysteresis on SWRC measurements (Bordoni et al., 2017; Hedayati et al., 2020; Iiyama, 2016; Pirone et al., 2014). It is worth mentioning that the current implementation of the PC<sub>NN</sub>-PTF ignores the effect of hysteresis since the lab measurements using HYPROP are made on the drying hydraulic path. We separately calculated the error terms for drying and wetting cycles to determine if PC<sub>NN</sub>-PTF performed better for drying than wetting data. However, we observed no difference between the two (data not shown here). This suggests that lab-based PTFs developed based on drying data do not necessarily work better for drying than wetting cycles in field conditions. Furthermore, Iiyama (2016) suggested that soil moisture hysteresis can be ignored in the field under dry conditions as numerous repetitions of wetting and drying cycles may have occurred while soil moisture remains within the routinely observed range. The same could be said for our study since the plots were maintained under deficit irrigation for extended periods (Haghverdi et al., 2021).

#### 3.2.2. Laboratory SWRCs

For the lab measurements using the HYPROP-WP4C system,  $PC_{NN}$ -PTF (RMSE=0.034 cm<sup>3</sup> cm<sup>-3</sup>) performed better than Rosetta (RMSE=0.063 cm<sup>3</sup> cm<sup>-3</sup>). A tendency to overestimate the VWC was observed for the  $PC_{NN}$ -PTF (MBE=0.022 cm<sup>3</sup> cm<sup>-3</sup>). A more pronounced underestimation was observed for Rosetta (MBE = -0.056 cm<sup>3</sup> cm<sup>-3</sup>), indicated by a high magnitude of negative bias. The correlation coefficient was greater than 0.90 for both models, showing an overall good agreement between the measured and the estimated VWC (Table 3). Larger and more complete databases with soil hydraulic properties measured with a standardized technique and uniform distribution of samples among soil classes should increase the predictive capability of a PTF (Vereecken et al., 2010). Since  $PC_{NN}$ -PTF is a machine learning approach, its performance is expected to improve as more soil hydraulic data measured with HYPROP experiments becomes publicly available for training the model.

The SWRCs estimated using the VG parameters obtained from the IM in HYDRUS-1D also showed reasonable accuracy with RMSE of 0.043 cm<sup>3</sup> cm<sup>-3</sup>, indicating comparable performance to Rosetta. A slight underestimation of the estimated VWC was observed (MBE =  $-0.007 \text{ cm}^3$  cm<sup>-3</sup>), which is also shown in Fig. 4. The agreement between the measured and estimated VWC was high (R=0.85) but lower than what was observed for the PC<sub>NN</sub>-PTF and Rosetta models (Table 3). In our study, all parameters of the VG model for SWRC were optimized using IM. Better results may be expected if parameters such as  $\theta_s$  and  $\theta_r$  are constrained within practical limits (Šimůnek et al., 1998a, 1998b). Nonetheless, results from our study indicate that in-situ SWRCs can serve as a reliable source for obtaining soil moisture information if labobtained SWRCs are not available.

## 3.3. Performance of PTFs at wet, intermediate, and dry tension regions of the SWRC

#### 3.3.1. In-Situ SWRCs

Table 4 shows the performance of PC<sub>NN</sub>-PTF and Rosetta for lab and in-situ measurements in three regions of the SWRC. In the wet range of the SWRC, PC<sub>NN</sub>-PTF (RMSE=0.008 cm<sup>3</sup> cm<sup>-3</sup>) performed better than Rosetta (RMSE=0.076 cm<sup>3</sup> cm<sup>-3</sup>) for the in-situ data. No considerable over or underestimation of the VWC was observed in the wet region by PC<sub>NN</sub>-PTF, whereas Rosetta underestimated at all the retention points (MBE = -0.76 cm<sup>3</sup> cm<sup>-3</sup>). Similarly, PC<sub>NN</sub>-PTF performed better in the intermediate region (RMSE=0.023 cm<sup>3</sup> cm<sup>-3</sup>) than Rosetta (RMSE=0.080 cm<sup>3</sup> cm<sup>-3</sup>). A slight tendency for overestimation of VWC was observed for the PC<sub>NN</sub>-PTF (MBE=-0.012 cm<sup>3</sup> cm<sup>-3</sup>), whereas underestimation was observed for Rosetta (MBE = -0.076 cm<sup>3</sup> cm<sup>-3</sup>) in the intermediate region. Both models showed comparable performance in the dry region of the SWRC, with PC<sub>NN</sub>-PTF performing slightly better

Table 3

Accuracy of the PC<sub>NN</sub>-PTFs, and Rosetta to estimate the laboratory and in-situ (May to September 2019) volumetric water content (cm<sup>3</sup> cm<sup>-3</sup>).

Lab measurements (HYPROP+WP4C)					In-situ me MPS6 + T	easurements DT (30 min)		In-situ measurements MPS6 + TDT (daily average)				
PC <sub>NN</sub> -PTF	RMSE	MAE	MBE	R	RMSE	MAE	MBE	R	RMSE	MAE	MBE	R
	0.034	0.029	0.022	0.94	0.048	0.034	-0.012	0.91	0.056	0.042	-0.029	0.91
Rosetta	0.063	0.057	-0.056	0.91	0.082	0.079	-0.079	0.90	0.084	0.081	-0.081	0.90

RMSE: Root mean square error (cm<sup>3</sup> cm<sup>-3</sup>), MAE: Mean absolute error (cm<sup>3</sup> cm<sup>-3</sup>), MBE: Mean biased error (cm<sup>3</sup> cm<sup>-3</sup>), R: Correlation coefficient.



Fig. 4. Scatterplots of measured and estimated volumetric water content using  $PC_{NN}$ -PTF, Rosetta, and inverse modeling via HYDRUS-1D for the lab and in-situ measured data. The solid blue line is the 1:1 line. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

#### Table 4

Performance of the  $PC_{NN}$ -PTF and Rosetta model to estimate the volumetric water content (cm<sup>3</sup> cm<sup>-3</sup>) for the laboratory and in-situ measurements at wet (pF $\leq$ 2) intermediate (2 < pF $\leq$ 3) and dry (pF>3) parts of the SWRC.

	PC <sub>NN</sub> -PT	F				Rosetta							
	Lab soil samples			In Situ measurements (30 min)			Lab soil samples			In Situ measurements (30 min)			
	pF≤2	$2 < pF \leq 3$	pF>3	pF≤2	$2 < pF \leq 3$	pF>3	pF≤2	$2 < pF \leq 3$	pF>3	pF≤2	$2 < pF \leq 3$	pF>3	
RMSE	0.038	0.030	0.026	0.008	0.023	0.083	0.061	0.070	0.027	0.076	0.080	0.087	
MAE	0.033	0.024	0.021	0.007	0.019	0.073	0.056	0.065	0.022	0.076	0.076	0.085	
MBE	0.028	0.017	-0.005	0.000	0.012	-0.073	-0.056	-0.065	-0.014	-0.076	-0.076	-0.085	
R	0.68	0.81	0.79	0.57	0.76	0.55	0.75	0.77	0.93	0.24	0.65	0.53	

RMSE: Root mean square error (cm<sup>3</sup> cm<sup>-3</sup>), MAE: Mean absolute error (cm<sup>3</sup> cm<sup>-3</sup>), MBE: Mean biased error (cm<sup>3</sup> cm<sup>-3</sup>), R: Correlation coefficient.

(RMSE=0.083 cm<sup>3</sup> cm<sup>-3</sup>) than Rosetta (RMSE=0.087 cm<sup>3</sup>cm<sup>-3</sup>). Both models underestimated the VWC in the dry region with MBE = -0.073 and -0.085 cm<sup>3</sup> cm<sup>-3</sup> for PC<sub>NN</sub>-PTF and Rosetta, respectively. R ranged from 0.55 in the dry region to 0.76 in the intermediate region for PC<sub>NN</sub>-PTF and from 0.24 in the wet region to 0.65 in the intermediate region for Rosetta.

#### 3.3.2. Laboratory SWRCs

For the lab-obtained SWRCs, the lowest performance for the  $PC_{NN}$ -PTF was observed in the wet region of SWRC (RMSE=0.038 cm<sup>3</sup> cm<sup>-3</sup>), where the model showed a tendency to overestimate the VWC for most of the soils (MBE=0.028 cm<sup>3</sup> cm<sup>-3</sup>) as also indicated in Fig. 4. The best performance was observed in the dry region (RMSE=0.026 cm<sup>3</sup> cm<sup>-3</sup>) followed by the intermediate region (RMSE=0.030 cm<sup>3</sup> cm<sup>-3</sup>). No substantial over or underestimation was observed in the dry range (MBE

= -0.005 cm<sup>3</sup> cm<sup>-3</sup>), whereas a slight overestimation of VWC was evident in the intermediate range (MBE=0.017 cm<sup>3</sup> cm<sup>-3</sup>). The R value was 0.68, 0.81, and 0.70 in the wet, intermediate, and dry regions of the SWRC, respectively. The better performance of PC<sub>NN</sub>-PTF in the intermediate and dry region of SWRC compared to the wet region can be attributed to the lack of measured retention points at soil saturation ( $\theta_s$ ) in the training dataset (Singh et al., 2020) and strong nonlinearity in the measured data close to saturation. Although laboratory-measured  $\theta_s$  is underestimated compared to the in-situ values because of incomplete saturation and air entrapment of the soil (Verbist et al., 2009; Wassar et al., 2016), overestimation in lab methods is also possible (Abbasi et al., 2003). The lack of measured data in the wet and dry regions of the SWRC can be addressed by including arbitrary data points to each soil sample of the training dataset as adopted by Haghverdi et al. (2018) by adding retention pair at oven-dry point (i.e., pF=6.8 and VWC=0 cm<sup>3</sup>

cm<sup>-3</sup>). These arbitrary points, such as  $\theta_s$  and  $\theta_r$  estimated from other PTFs, can further enhance the performance of PC<sub>NN</sub>-PTF when training data sets are limited.

For Rosetta, the lowest performance was observed in the intermediate region of SWRC (RMSE=0.070 cm<sup>3</sup> cm<sup>-3</sup>), where the model tended to underestimate soil moisture (MBE =  $-0.065 \text{ cm}^3 \text{ cm}^{-3}$ ). The best performance was observed in the dry region (RMSE= $0.027 \text{ cm}^3 \text{ cm}^{-3}$ ) followed by the wet range (RMSE= $0.061 \text{ cm}^3 \text{ cm}^{-3}$ ). Underestimation was observed in both the dry (MBE =  $-0.014 \text{ cm}^3 \text{ cm}^{-3}$ ) and wet (MBE =  $-0.056 \text{ cm}^3 \text{ cm}^{-3}$ ) regions but was less pronounced compared to the intermediate region. The best agreement between the observed and estimated VWC was in the dry region, reflected by R value of 0.93, followed by the intermediate and wet regions with R values of 0.77 and 0.75, respectively (Table 4).

As per the SWRCs obtained from the IM (Table 5), the lowest performance was observed in the dry region (RMSE=0.071 cm<sup>3</sup> cm<sup>-3</sup>), followed by the wet region (RMSE=0.042 cm<sup>3</sup> cm<sup>-3</sup>). The best performance was observed in the intermediate region (RMSE=0.036 cm<sup>3</sup> cm<sup>-3</sup>) and with slight overestimation, as indicated by MBE of 0.014 cm<sup>3</sup> cm<sup>-3</sup>. Underestimation of the VWC was observed in the wet region (MBE = -0.031 cm<sup>3</sup> cm<sup>-3</sup>), whereas overestimation was observed in the dry region (MBE=0.063 cm<sup>3</sup> cm<sup>-3</sup>), as reflected in Fig. 4, where most of the data points are above the 1:1 line at lower VWC and below the line at the higher values of VWC.

# 3.4. Novelty and limitations of this study and directions for future research

The novelty of this work was threefold. Firstly, we addressed a research gap by comparing in-situ soil water retention measurements with HYPROP-WP4C measurements and HYPROP-based PC<sub>NN</sub>-PTF estimations of the SWRC. Secondly, we utilized calibrated sensor measurements to create a comprehensive field-based soil tension and water content dataset for inverse modeling of the SWRC using HYDRUS-1D. Thirdly, we developed the first web application for estimating the SWRC using the PC<sub>NN</sub>-PTF approach.

This study only focused on measuring and estimating SWRC. We recommend further studies to investigate the differences between soil hydraulic conductivity curves obtained in the lab versus field measurements and evaluate the performance of hydraulic conductivity PTFs such as the PC<sub>NN</sub>-PTF developed by Singh et al. (2021) for new soils and under field conditions.

The HYPROP-WP4C system, similar to other standard laboratory

#### Table 5

Performance of the van Genuchten model parametrized using inverse modeling of the in-situ soil moisture data.

HYDRUS-1D (Inverse Modeling) vs Lab											
Plot	RMSE	MAE	MBE	R							
39–3	0.055	0.047	-0.037	0.90							
39–7	0.046	0.038	0.017	0.96							
44–3	0.042	0.035	0.021	0.96							
44–7	0.038	0.033	-0.007	0.83							
49–3	0.028	0.025	-0.003	0.97							
49–7	0.029	0.025	0.003	0.95							
56–3	0.046	0.039	0.001	0.95							
62–3	0.048	0.041	-0.026	0.99							
62–7	0.038	0.031	-0.02	0.99							
66–3	0.035	0.029	0.017	0.99							
66–7	0.053	0.05	-0.043	0.98							
For different regions of the SWRC											
pF≤2	0.042	0.036	-0.031	0.57							
$2 < pF{\leq}3$	0.036	0.030	0.014	0.58							
pF>3	0.071	0.063	0.063	0.66							

RMSE: Root mean square error (\*\* $cm^3 cm^{-3}$ ), MAE: Mean absolute error ( $cm^3 cm^{-3}$ ), MBE: Mean biased error ( $cm^3 cm^{-3}$ ), R: Correlation coefficient.

techniques, only measured the main drying SWRC, while sensor pairing in the field captures both drying and wetting branches of the SWRC. We showed that the HYPROP-based  $PC_{NN}$ -PTF can provide a reasonable estimation of soil water retention under field conditions, albeit at lower accuracy than laboratory data. Cautions should be made, however, for future field applications since  $PC_{NN}$ -PTF only estimates the main drying curve, while field data encompass wetting and drying cycles. Therefore, we recommend that future lab-based PTFs be developed to estimate both main drying and wetting curves (as the upper and lower bounds) to better capture soil moisture dynamics under natural field conditions. In addition, we leave it to future research to determine if new sets of PTFs could be developed based on field data and sensor pairing techniques.

A limitation of the MPS6 sensor is its requirement for equilibrium to provide soil tension measurements, which may not correspond to instantaneous TDT-based soil moisture measurements. This may impact sensor pairing data when soil moisture changes in short timestamps, such as during irrigation events. Additionally, MPS6 sensors did not capture the very wet soil condition close to saturation since it is outside the sensor's measurement range.

We did not consider hysteresis during inverse modeling and leave it to future research to determine whether that could enhance the performance of the inverse modeling approach using HYDRUS-1D.

#### 4. Conclusion

In this study, the PC<sub>NN</sub>-PTF approach was employed to estimate the complete soil water retention curve (SWRC) using soil texture (SSC) and bulk density (BD). The PC<sub>NN</sub>-PTF was trained using a combination of previously published international and Turkish datasets, all measured through evaporation experiments and HYPROP. The HYPROP system offers the advantage of providing a quasi-continuous description of the retention function within the tensiometric moisture range (up to pF 3), with dry-end (pF>4) measurements obtained using the WP4C Dew Point PotentioMeter. Our PC<sub>NN</sub>-PTF demonstrated superior performance compared to Rosetta in estimating soil water content data in both laboratory settings and field conditions. Particularly for in-situ soil moisture measurements, PC<sub>NN</sub>-PTF provided a more accurate estimation of SWRC than Rosetta in the intermediate region, although caution is advised in the wet region. Inverse modeling of VG parameters from insitu soil moisture data reasonably estimated VWC in the intermediate region. Unlike the HYPROP-WP4C system, the in-situ SWRCs created in this study did not cover the entire soil moisture range from saturation to dryness, mainly due to limitations in the measurement range of soil moisture sensors. Field data also exhibited more scattering, primarily attributed to hysteresis induced by wetting and drying cycles. Nevertheless, field sensors are increasingly used due to advancements in irrigation technology, generating substantial data. Therefore, it is crucial to explore the utility of directly using field-collected data for soil hydrological estimations. Our results indicate that PC<sub>NN</sub>-PTF could serve as an essential tool for future research in this direction.

#### CRediT authorship contribution statement

Amninder Singh: Writing – review & editing, Writing – original draft, Methodology, Formal analysis, Data curation, Conceptualization. Amir Verdi: Writing – review & editing, Writing – original draft, Supervision, Resources, Project administration, Methodology, Investigation, Funding acquisition, Data curation, Conceptualization.

#### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

#### Data availability

Data will be made available on request.

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