J. Hydrol. Hydromech., 72, 2024, 3, 312–335
https://doi.org/10.2478/johh-2024-0013

sciendo Journal of Hydrology and Hydromechanics Institute of Hydrology SAS

Functional evaluation of different soil hydraulic parametrizations in hydrological simulations reveals different model efficiency for soil moisture and water budget

Zsolt Kozma[1,2*], Bence Decsi[1,2], Tamás Ács[1,2], Zsolt Jolánkai[1,2], Miklós Manninger[3], Norbert Móricz[3], Gábor Illés[3], Gyöngyi Barna[4,5], András Makó[4,5], Brigitta Szabó[4,5]

[1] Budapest University of Technology and Economics, Faculty of Civil Engineering, Department of Sanitary and Environmental Engineering, Műegyetem rkp. 3. H-1111 Budapest, Hungary.
[2] National Laboratory for Water Science and Water Security, Budapest University of Technology and Economics, Faculty of Civil Engineering, Department of Sanitary and Environmental Engineering, Műegyetem rkp. 3. H-1111 Budapest, Hungary.
[3] University of Sopron, Forest Research Institute, Department of Ecology and Forest Management, Várkerület 30/A, H-9600 Sárvár, Hungary.
[4] Institute for Soil Sciences, HUN-REN Centre for Agricultural and Environmental Research, Herman Ottó út 15. H-1022 Budapest, Hungary.
[5] National Laboratory for Water Science and Water Security, Institute for Soil Sciences, HUN-REN Centre for Agricultural and Environmental Research, Herman Ottó út 15. H-1022 Budapest, Hungary.
[*] Corresponding author. Tel.: +36-20-4964745. E-mail: kozma.zsolt@emk.bme.hu

Abstract: Novel soil datasets and the application of pedotransfer functions provide soil hydraulic input data for modelling hydrological processes at different scales. We aimed to evaluate the reliability of soil hydraulic parameters derived by indirect methods in simulation of soil moisture time series and water budgets at profile level of three sites (Forest, Orchard and Grassland) from a Central European catchment (Lake Balaton, Hungary). Five soil-vegetation-atmosphere model variants were set up with the Hydrus-1D model for each site, differing only in the parametrization of input soil data: i) a calibrated reference, ii) measured values, iii) values predicted from measured basic soil properties, iv) values predicted from national soil map information, v) values derived from the 3D soil hydraulic dataset of Europe. Calibrated soil parameters led to Nash-Sutcliffe efficiency 0.50, 0.54 and 0.71 for the Forest, Orchard and Grassland Site respectively. The outcomes for model efficiency of soil moisture underline the superiority of local databases over regional ones and the need for more detailed vertical discretization during modelling. The model performance according to soil moisture and water budget accuracy led to different rank order of model variants. Water budget comparisons indicated moderate differences between the hydrologic fluxes simulated by the different model variants, emphasizing the uncertainties associated with soil hydraulic parametrization either at local or at watershed scale.

Keywords: Pedotransfer function; Hydrus-1D; Soil hydraulic properties; Soil moisture dynamics; Water budget.

INTRODUCTION

The input data requirement of hydrological, water quality and ecological models poses a growing challenge (Arnold et al., 2012; Farkas et al., 2011; Trodahl et al., 2017; Van Looy et al., 2017). This data need is expected to further increase in the future with the development of the theoretical background, the computational capacity and the achievable spatial resolution (Vereecken et al., 2016). Remote sensing (Karimi and Bastiaanssen, 2015; Mohanty et al., 2017) and automated hydrometeorological monitoring (Dorigo et al., 2013; Fiala et al., 2014; Ganot et al., 2017; Qu et al., 2016) go through remarkable technological advancement, resulting in improving temporal and spatial resolution. However, these methods provide mostly only indirect information about the physical characteristics of the subsurface domain/region. Thus, soil hydraulic parametrization, namely the definition of the soil moisture retention curve (MRC) and hydraulic conductivity curve (HCC) became one of the main challenges of process based hydrologic/environmental modelling both at local and catchment scale (Đukić et al., 2021; Kozma et al., 2022; Vereecken et al., 2016). Direct measurement of these soil hydraulic properties is time consuming and costly, therefore in many cases they are estimated with pedotransfer functions (PTFs) from easily measurable soil properties (e.g. texture, bulk density). In most of the model studies, the parameters of the MRC and the HCC are calculated using linear regression or machine learning-based PTFs, based on soil texture, organic carbon content, and bulk density (Van Looy et al., 2017). Recognizing the situation, novel soil hydraulic databases were recently developed with different methodologies, spatial characteristics and coverage (point or spatial datasets, various resolution, national, continental or global) e.g. among others (Chaney et al., 2016; Dai et al., 2019; Gupta et al., 2022; Orgiazzi et al., 2018; Pásztor et al., 2020; Poggio et al., 2021; Rahmati et al., 2018; Soil Survey Staff Natural Resources Conservation Service United States Department of Agriculture, 2020; Tóth et al., 2017; Weynants et al., 2013).

The reliability of hydraulic data sets generated from these soil hydraulic databases, i.e. to what extent do they improve the results of environmental modelling, for example the simulation of soil moisture, are rarely analysed by using measured field data. Usually soil hydrologic data sets are compared against each other through model applications (Nemes et al., 2003; Vereecken et al., 1992; Zhao et al., 2018). As certain model inputs, the hydraulic data sets based on different data sources are evaluated usually separately (a single dataset per study) and/or indirectly (comparing measured and simulated state variables, which are indirectly affected by soil hydraulic parameters) (Ganot et al., 2017; Kozma et al., 2014; Scanlon et al., 2002).

Ganot et al. (2017) indirectly proved the reliability of the European pedotransfer functions (EU-PTF-s, Tóth et al., 2015), by using seepage hydraulic simulations they modelled the effects of an artificial recharge lake on groundwater levels. The soil hydraulic parametrization of the involved soil layers was determined by using a number of widespread datasets. Those results provided the best agreement between measured and simulated groundwater levels, which were based on the EU-PTF-s. Scanlon et al. (2002) demonstrated that benchmarking soil water movement simulation results and measured soil moisture data provides valuable information about the uncertainty related to theoretical considerations, model algorithms and input data. Nemes et al. (2003) compared the performance of soil water content (WC) simulations using parameters of the soil moisture retention curve estimated with national and international PTFs. In their study the differences in the accuracy of simulations were marginal, even if measured soil hydraulic properties were considered. Thus, computing soil hydraulic properties with international PTFs were found to be an alternative solution compared to using national PTFs or measured values. Guber et al. (2009) found that using several PTFs in a multi-model ensemble can enhance simulation of vertical water flow under field conditions. In their study the geographic similarity of the PTFs' training set did not influence the performance of the hydraulic model, however they used different PTFs for the prediction of only the van Genuchten parameters (van Genuchten, 1980) to describe the MRC, the saturated hydraulic conductivity (KS) was computed with a single PTF for all model variants. Loosvelt et al. (2011) analysed whether the type of PTFs – used to compute soil hydraulic parameters – influences simulation of soil water content. They found that region specific PTFs are preferable over non-region specific PTFs to assess the uncertainty of modelled soil water content. Nasta et al. (2021b) compared the predictive capability of several PTFs on European soil hydrological datasets and analysed the performance of the best performing ones in simulating the water balance components of a transect. Based on their results estimation of KS had high uncertainty with all analysed PTFs, which influence soil water storage simulations. These findings underpin the importance of quantifying the potentials and limitations of applying predicted soil hydraulic properties in water flow simulations.

Our assumption was that comparative hydrological model studies designed in the fashion of the above mentioned are suitable to evaluate the soil hydraulic data derived from different sources. In this study our aim was to analyse the reliability of derived soil hydraulic data sets for simulating soil moisture time series and water budget at soil profile scale. All of the five tested soil hydrologic datasets provide the Mualem-van Genuchten (MVG) parameters of the MRC and the HCC. We used the Hydrus-1D software (Šimůnek et al., 2013) to carry out simulations at three monitoring sites (Lake Balaton catchment area, Hungary), where measured hydro-meteorological and soil moisture data were available.

MATERIALS AND METHODS

Basic concept

To evaluate the reliability of the analysed soil hydraulic datasets, we carried out process based hydrologic simulations at local scale. The analysis followed the logic below:

(1) The water content and water budget of a monitored soil profile can be described with a series of similar soil-vegetation-atmosphere (SVAT, Vereecken et al. (2016)) model variants, differing only in their soil hydraulic parametrization (depths of soil layers, MVG parameters of the MRC and HCC).

(2) Presumably, these nearly identical models will lead to different agreement between measured and simulated soil moisture time series. Also, they provide varying estimates of water budget components.

(3) If the quality of the input data used for boundary conditions is sufficiently good for modelling purposes (accurate local information with multi-season, continuous temporal coverage), then we can assume that the goodness-of-fit of the model variants indicate the reliability of the underlying indirectly derived soil data.

(4) The (1)–(3) steps can be considered as a comparative, functional evaluation of the studied soil hydraulic databases at pointwise/local scale. The more sites are involved in the assessment the more extensive information it provides.

For model performance evaluation we compared the accuracy of (i) the modelled soil water content time series using common model efficiency measures and (ii) the components of the simulated water budgets. The previous is mainly defining at detailed local, site-specific analyses, while the latter one is also relevant for distributed parameter catchment scale modelling, as it quantifies the effect of soil information on the hydrological response of soil profiles. Soil water simulations at local (plot, hillslope) scale are very sensitive to soil hydraulic properties, especially to saturated WC, field capacity and KS (Nasta et al., 2021a). KS governs infiltration and runoff generation, while saturated WC and field capacity has impact e.g. on the recession of the soil moisture curve during dry periods. Hydrological calculations at catchment scale are also highly influenced by soil hydraulic parameterization (Zhao et al., 2024).

Study sites

We performed the analysis at three locations: at two hydro-meteorological monitoring sites of the Forest Research Institute of the University of Sopron in Fiad and Szalafő and one monitoring site in Keszthely (Figure 1). Basic soil and climatic properties are highlighted in Table 1.

The mixed oak-beech Forest Site is in Fiad, which is situated in the central part of the Trans-Danubian region of Hungary, South to the Lake Balaton (46°37'18.0" N, 17°49'48.6" E, 210 m a.s.l.) (Figure A1). The site is located in zonal situation without the effect of slopes and surplus water. The soil type is Endocalcaric Cambisol (Pantoloamic, Ochric, Bathycalcic) (IUSS Working Group WRB, 2015). Soil water content is monitored with Decagon ECH20 EC-5 (Meter Group Inc., USA) sensors at 10, 20, 30, 50 and 100 cm soil depths at every 15 minutes. Meteorological data is available from two nearby meteorological stations.

The Orchard Site is in Keszthely, on the Western shore of Lake Balaton (46° 44' 46.43" N, 17° 14' 19.31" E, 116 m a.s.l.) (Figure A2). Pear trees are grown in uniform rows, with mowed, spontaneous grass flora covering the alleys. The soil is Cambic Endocalcic Phaeozem (Aric, Pantoloamic) on loess parent material. Soil water content is measured with FP/mts probe of the TDR/MUX/mpts meter (Easy Test) at 15, 25, 35, 45, 55, 65 and 95 cm soil depth at every hour (Skierucha et al., 2006). Meteorological time series for the site is available from a close-by meteorological station.

The Grassland Site is located in Szalafő, in the Upper Zala Valley (46° 51' 17.0" N, 16° 22' 28.0" E, 257 m a.s.l.) (Figure A3).

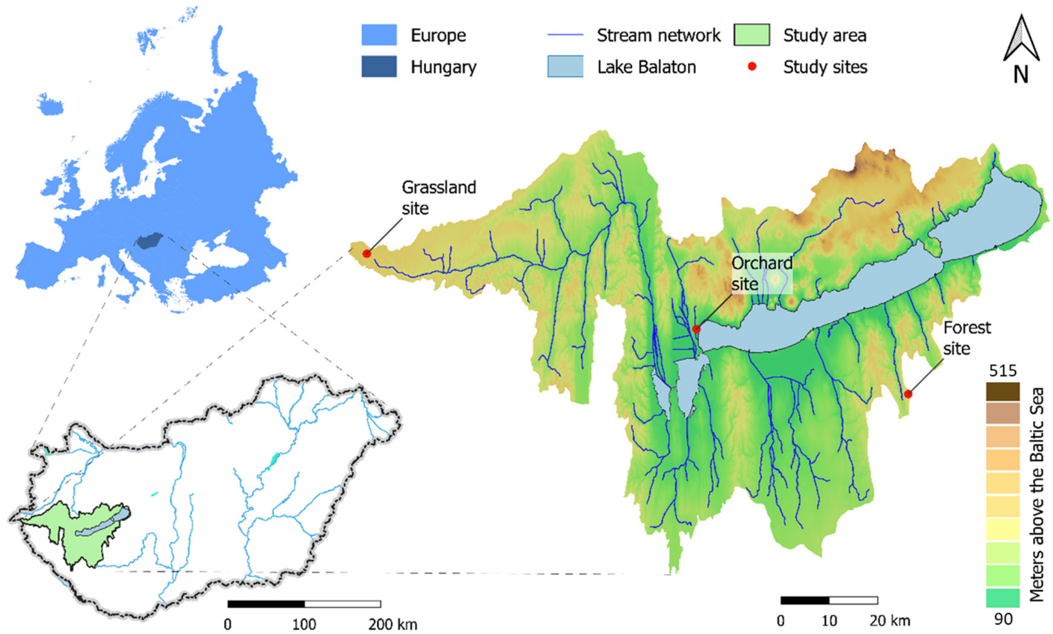


Fig. 1. Overview of the Lake Balaton catchment and the three sites: Forest Site (Fiad); Orchard Site (Keszthely); Grassland Site (Szalafő).

Table 1. Soil and meteorological properties and the studied soil profiles. Meteorological data refers to the period 2002-2021 (Hungarian Meteorological Service, 2022). Abbreviations: WRB SRG: WRB Soil Reference Group; SOM: Soil Organic Material; EC: Electrical Conductivity. P_{sum}: annual precipitation sum; T_{mean}: annual mean air temperature.

Soil profile name	Depth (cm)	Clay (%)	Silt (%)	Sand (%)	Texture	SOM (%)	$CaCO_3$ (%)	$pH_{\_H2O}$	EC 1:2.5 (µS/cm)	Climate P_{sum};T_{ave} (C; mm)
Forest Site Fiad	0–15	16.73	62.37	20.90	silt loam	3.47	0.08	6.09	158	moderately warm, moderately wet 638 mm 11.0°C
	15–40	25.56	52.99	21.45	silt loam	0.86	0.06	5.57	44.5	
	40–75	27.57	50.81	21.63	clay loam	0.62	0.08	6.01	36.5	
	75–110	17.54	59.62	22.85	silt loam	0.59	24.26	8.27	160.5	
	110–130	13.40	61.15	25.45	silt loam	0.38	29.67	8.45	146	
Orchard Site Keszthely	0–20	20.40	33.08	46.52	loam	1.48	0.39	7.79	177	moderately warm, moderately wet 623 mm 11.1°C
	20–40	20.04	32.47	47.49	loam	1.10	0.21	7.89	143.5	
	40–80	20.65	31.84	47.51	loam	0.90	0.38	8.01	151	
	80–140	19.20	53.80	27.00	silt loam	0.53	30.16	8.44	143.5	
Grassland Site Szalafő	0–15	11.03	69.54	19.43	silt loam	4.81	0.08	7.11	242	moderately cool and wet 747 mm 10.3°C
	20–50	16.40	64.51	19.09	silt loam	1.63	0.08	7.12	119	
	50–65	25.14	59.87	14.99	silt loam	0.75	0.04	7.14	105	
	65–80	29.97	50.97	19.06	silty clay loam	0.45	0.10	6.83	132.5	
	100–120	31.73	56.40	11.87	silty clay loam	0.27	0.02	5.81	94	

Soil type is Cambic Luvic Katostagnic Chernic Phaeozem (Endodensic, Episiltic, Katoloamic) developed on a sandy, clayey, marly Pannonian sediment. Campbell CS616 sensors (Campbell Scientific, 2020) are used to monitor soil water content at 10, 20 and 40 cm depth at every 10 minutes, of which daily aggregated values were considered for the analysis. Meteorological parameters were measured at the site.

In case of all three sites, daily averages/sums of precipitation, air temperature, relative humidity, wind speed, global radiation and soil moisture time series were used for the simulations. The soil moisture sensors have been installed after using standard calibration with bulk EC of ≤ 0.5 dS m^{-1}, bulk density of ≤ 1.55 g cm^{-3}, and measurement range of 0% to 50% volumetric WC. Post installation calibration with gravimetric method has also been carried out for each soil horizons. The derived calibration equations were applied on the time series soil moisture data.

Accuracy of the sensors were ±2%. The 10-min/15-min/1-hour step soil moisture measurements were inspected visually to identify and filter erroneous readings. This was done according to Dorigo et al. (2013) and gaps, spikes, oversaturation periods, geophysical consistency were checked. The filtered sub-daily soil moisture data were averaged to gain daily means at all sites. Finally, periods of low soil temperatures ($T_{soil,daily}$ < 5 °C for the Forest and Orchard, $T_{soil,daily}$ < 10 °C for the Grassland) were excluded in order to minimize the measurement uncertainty caused by the temperature effect on the soil moisture sensors.

During excavating the soil profiles, from every soil horizon disturbed and six parallel undisturbed samples were taken. Undisturbed soil cores have 5 cm high and 5 cm diameter. Soil physical and chemical properties, water retention characteristics and saturated hydraulic conductivity were measured according to the Hungarian standard (MSZ-08.0205:1978, 1978; Buzás, 1988, 1993). Water retention between 1 and 50 kPa was determined on three 100 cm³ undisturbed samples for each horizon, using the hanging water column method with sand- and kaolin-plate boxes. For pressures between 250 and 1500 kPa, pressure chambers were used on 2 cm³ disturbed samples. Saturated hydraulic conductivity was measured using the falling head method on three 100 cm³ undisturbed samples for each horizon. Finally, geometric mean values were calculated for the three-three repetitions of each horizon. The graphs in Figure A4 show the measured pF-water content data pairs and the fitted MRC-s for all sampled profiles.

Soil-vegetation-atmosphere model – theoretical background

To describe water movement in the soil profiles, we considered the following hydrological processes for all sites: interception, evapotranspiration (ET) and water stress limited root water uptake, snow hydrology, surface runoff and single porosity matrix flow.

Soil water movement was simulated by the numerical solution of the (1) Richards equation. We used the (2)–(4) MVG equations to approximate the MRC and HCC. The MVG equations are among the most widespread closed form relationships for this purpose (Nimmo, 2009). Also, most soil hydraulic data sets provide information by giving the spatially variable parameter values for these functions.

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial x}\left[k(h)\left(\frac{\partial h}{\partial x} + 1\right)\right] - S(h) \tag{1}$$

$$\theta(h) = \begin{cases} \theta_r + \dfrac{\theta_s - \theta_r}{[1 + |\alpha \cdot h|^n]^m}, & h < 0 \\ \theta_s, & h \geq 0 \end{cases} \tag{2}$$

$$k(h) = k_0 \cdot S_e^l \left[1 - \left(1 - S_e^{\frac{l}{m}}\right)^m\right]^2 \tag{3}$$

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} \tag{4}$$

where θ(h) is the water content of the soil (cm^3 cm^{-3}) at a given h matric pressure head (expressed in cm of water column); θ_r is the residual water content (cm^3 cm^{-3}); θ_s is the saturated water content (cm^3 cm^{-3}); α (cm^{-1}), n (–), and m (–) are fitting parameters, where m = 1 – 1/n; k(h) is the soil hydraulic conductivity (cm day^{-1}) at h; k_0 is the hydraulic conductivity acting as a matching point at saturation (cm day^{-1}); S_e is the effective saturation (–) and l is a fitting parameter related to tortuosity of the pore space (–).

Soil-vegetation-atmosphere model – practical setup

To implement the SVAT approach, we mainly relied on the Hydrus-1D software (Šimůnek et al., 2013). The Hydrus code is a widely applied numerical solver to describe water movement in variably saturated soil profiles. It provides versatile, stable and reliable solution of challenging unsaturated phenomena with a strong emphasis on soil hydraulic parametrization. However, in case of the Forest Site we also applied the Brook90 model (Federer, 2021). The model setups for the three sites were similar in many aspects, but there were also some major differences. We introduce these by going through model geometry, initial and boundary conditions, description of vegetation (Figures A1–3).

The depth of the model domains was selected with respect to the results of soil profile surveys. In each model version, we adjusted the soil layers with respect to the actual soil hydrological databases (see below). Daily soil moisture data was used at the observation points during the calibration-validation process in case of all three sites.

Initial conditions were estimated with respect to the measured water contents and a two-month warm-up period was also applied. The soil profile surveys showed that neither the groundwater table nor the capillary fringe reach the domain of interest, so we uniformly used a zero-gradient lower boundary condition (free drainage). Considering the terrain, surface runoff was allowed at all sites.

Measured daily meteorological data were used to define the upper boundary condition time series. The amount of precipitation (rain or snow) was reduced with interception. Potential evapotranspiration (PET) was computed with the Penman-Monteith formula (Monteith, 1965). The built-in vegetation functions (interception, light extinction, potential evapotranspiration, root water uptake) of Hydrus-1D can facilitate mainly agricultural crops, but not forests. For the latter, the Brook90 software (Federer, 2021) is a suitable alternative, as this model was developed to describe hydrological processes with more focus on canopy processes. It provides a better approximation of interception, potential and actual ET and infiltration in case of wooded areas. Thus in case of Forest Site the Brook90 was used to calculate elements of the canopy related water budget, then these time series were used in the Hydrus-1D as atmospheric boundary conditions.

Parametrization of the vegetation properties was based both on field observations and literature data. The maximal leaf area index (LAI) of the mixed oak/beech forest at Fiad was determined with leaf sampling (using five pieces of 0.25 m^2 frames, according to Bréda, (2003)), while the seasonal changes of LAI were estimated by using MODIS 16-day composite NDVI images (Wang et al., 2005). At the Orchard and Grassland Sites the variation of LAI was unknown as the grass was mowed according to an irregular and unrecorded schedule. Thus we assumed a trapezoid type of time series (Figure A5), of which the shape was partially based on Breuer et al. (2003), partially manually adjusted. Maximal rooting depth was set to 150 and 60 cm for the Forest and Grassland Site respectively, while the root distribution was based on field observations and calibration. The water stress of root water uptake was modelled with the S-shape function (calibrated parameters) (Wesseling et al., 1991) for the Forest Site and with the Feddes-formula (default parameters for pastures) for the Orchard and Grassland Sites (Feddes et al., 1978).

Applied soil hydraulic parameter sets

The model variants differed only in the depth intervals of soil layers and the parameterization of the MRC and HCC. If it is possible in practice, water content-pressure head data pairs and

KS are measured to derive hydraulic parameters for soil hydrological simulations. For the description of the MRC, parameters of the van Genuchten model are fitted on the water content-head data pairs. There were no available k-h data pairs to optimize the k_0 and l parameters, therefore we used measured KS as a matching point, and l = 0.5 as a common default value in of the MVG model based on (Mualem, 1976). Despite that this is not the most accurate approach regarding the description of the hydraulic conductivity, it is widely used due to the high cost of measuring unsaturated hydraulic conductivity.

The five model variants for soil hydraulic properties were (1) reference (REF), (2) measured in the laboratory (MEAS_SHP), (3) predicted from the measured basic soil properties with the class European hydraulic pedotransfer functions (Tóth et al., 2015) (MEAS_EU-PTF), (4) mapped with the EU-PTFs based on the national 100 m resolution DOSoReMI.hu soil dataset (Pásztor et al., 2020) (HUN-MAP_EU-PTF), (5) retrieved from the 250 m resolution EU-SoilHydroGrids dataset (Tóth et al., 2017) (EU-SHG). The REF model variant was derived based on field and laboratory measured data, from which some were modified during the calibration-validation process. We considered this variant as the best achievable approximation of the soil water contents and fluxes computed by the Hydrus-1D simulation. The data sources used in the five model versions are summarized in Table 2.

For the HUN-MAP_EU-PTF we computed the soil hydraulic parameters for the 0–30, 30–60 and 60–90 cm soil depths at a 100 m horizontal resolution for the whole Balaton catchment and extracted the parameters from those maps for the locations of the analysed soil profiles. As part of the mapping process we analysed the performance of soil hydraulic maps – HUN-MAP_EU-PTF and EU-SHG – based on the Hungarian Detailed Soil Hydro-physical Database (Makó et al., 2010). The dataset includes measured soil hydraulic data of soil profiles located at the Balaton catchment. For calculating the residuals between the mapped and measured properties, we harmonized the soil water retention values of the soil hydro-physical dataset for the soil depths used on the maps, i.e. 0–30, 30–60, 60–90 cm (HUN-MAP_EU-PTF) and 0–2.5, 2.5–10, 10–22.5, 22.5–45, 45–80, 80–150, 150–200 cm (EU-SHG) by using mass-preserving splines built in the R package GSIF (Hengl, 2017). The performance of the maps was evaluated based on mean error (ME) and root mean square error (RMSE) values. For the comparison of HUN-MAP-EU-PTF and EU-SHG maps the Kruskal–Wallis test of the R package "agricolae" (De Mendiburu, 2017) was applied at the 5% significance level on the mean square error values. The analysis related to the maps were performed in R (R Core Team, 2019)

Calibration-validation and model performance comparison

Automated calibration was applied only for the REF. Standard measures of goodness-of-fit (coefficient of determination – R^2, mean absolute error – ME, root mean square error – RMSE, Nash-Sutcliffe Model Efficiency – NSME, see formulas in the Appendix) were used to quantify the agreement between measured and simulated soil moisture time series (Nash and Sutcliffe, 1970). Considering the evaluation of goodness-of-fit, we followed the general guidance of Harmel et al. (2018). NSME was used as the primary efficiency indicator. We considered the simulation results unacceptable, if NSME was negative, satisfactory, if NSME > 0.5 and good if NSME > 0.66. We continued the calibration-validation process at least until the NSME was above 0.5 for the whole period. As the efficiency order of the non-calibrated model variants varied from site to site, we also calculated an overall rank to summarize the model reliability for all three sites. Here (i) we set up the rank (1 – best; 5 – worst) of the model variants according to the order of their efficiency indicators for the given site, then (ii) averaged the ranks for the three sites, giving an extra penalty rank point for negative NSME values to express the low reliability of such results.

Table 2. The source of soil depth intervals and soil hydraulic parameters input data used for the soil profile simulations.

Name of model variant	Source of the input data		Figure for vertical profile of soil hydraulic parameters
	Soil depth intervals	MVG and KS parameters	
REF	Measured and calibrated	Measured and calibrated	Forest: Fig A1 (1) Orchard: Fig A2 (1) Grassland: Fig A3 (1)
MEAS_SHP	Measured	Measured	Forest: Fig A1 (2) Orchard: Fig A2 (2) Grassland: Fig A3 (2)
MEAS_EU-PTF	Measured	Predicted from the measured easily available soil properties (particle size distribution, organic carbon content, topsoil/subsoil distinction, bulk density, pH) with the European pedotransfer functions (EU-PTFs) with PTF22 (MRC) and PTF16 (KS) of EU-PTFs	Forest: Fig A1 (3) Orchard: Fig A2 (3) Grassland: Fig A3 (3)
HUN-MAP_EU-PTF	0–30, 30–60, 60–90 cm DOSoReMI.hu	Predicted based on soil data of the DOSoReMI.hu maps with PTF19 (MRC) and PTF16 (KS) of EU-PTFs	Forest: Fig A1 (4) Orchard: Fig A2 (4) Grassland: Fig A3 (4)
EU_SHG	0–2.5, 2.5–10, 10–22.5, 22.5–45, 45–80, 80–150, 150–200 cm EU-SoilHydroGrids	Derived from EU-SoilHydroGrids maps	Forest: Fig A1 (5) Orchard: Fig A2 (5) Grassland: Fig A3 (5)

The calibration involved the following parameters and variables: (i) vertical position of the soil layers, (ii) soil hydraulic parameters (for all layers), and (iii) vegetation parameters (extinction and interception coefficients, shape of LAI time series, vertical distribution of root density). Furthermore, in the REF variant we used an additional thin virtual soil layer at the surface to represent the effects of the sensitive boundary domain, i.e. higher organic material content and root density, possible presence of macro-pores, thus enhanced infiltration.

Considering the water budget, only open field precipitation was measured directly among the governing hydrological processes, while PET was estimated independently prior to the simulations. All other water balance components were calculated as part of the model simulations. Thus – in the absence of a complete measured dataset – we used the simulated annual water budget of the calibrated REF model as the reference scenario for the model variant comparison for all three sites.

RESULTS

Soil hydraulic properties

The RMSE values of the MRC computed based on the mapped van Genuchten parameters are 0.07 cm^3 cm^{-3} for HUN-MAP_EU-PTF and 0.07–0.09 cm^3 cm^{-3} for EU-SHG (Table 3.) analysed on the samples with measured theta-head pairs of Balaton catchment. Based on the Kruskal-Wallis test, HUN-MAP_EU-PTF performed significantly better than EU-SHG based on the mean squared error of the predictions. During deriving the parametric EU-PTFs, the RMSE was 0.058–0.067 cm^3 cm^{-3} for the class PTFs (PTF19) (Tóth et al., 2015), which is comparable with the RMSE of HUN-MAP_EU-PTF. In case of both maps PTF16 of EU-PTFs was used to compute the KS. For $\log_{10}$KS the PTF16 had 1.06–1.09 $\log_{10}$ (cm day^{-1}) RMSE on the test set of EU-PTFs. For HUN-MAP_EU-PTF the RMSE was 0.86–1.06 $\log_{10}$ (cm day^{-1}), for EU-SHG it was larger than that, but there was no significant difference between the performance of the two maps, however it could be analysed at only maximum 37 samples per soil horizons. It was expected that the performance of the mapped soil hydraulic properties would decrease compared to that of the PTFs, due to the uncertainty of soil property maps, which were used as input information for the predictions. The RMSE values of the derived maps are comparable with the findings of Zhang et al. (2018), Gupta et al. (2021), and Gupta et al. (2022).

Figure A9 and Figure A10 show the density plots of mapped values in the case of HUN-MAP_EU-PTF and EU-SHG model variants computed for the Balaton catchment. The density plots of the soil hydraulic parameters have multiple peaks within the same soil depth, because for HUN-MAP_EU-PTF, the parameters of MRC were computed with class PTF, which considers USDA texture classes and topsoil/subsoil distinction. Majority of the residual water content values is zero, which is in line with findings of Zhang et al. (2022). The KS was computed with regression-tree-based PTF (PTF16) for both maps.

For each site, the five soil profiles derived from (i) calibration, (ii) measurements of field samples, (iii) from measured basic soil properties with PTF and (iv-v) from using soil maps are presented in the Appendix (Figure A1–3). The horizontal characteristics of the gravitational, plant available, unavailable water content and solid part are similar for the measured soil hydraulic properties (MEAS_SHP) and predicted ones from measured basic soil properties (MEAS_EU-PTF). In the case of mapped soil hydraulic properties (HUN-MAP_EU-PTF, EU_SHG) data shows decrease in porosity – i.e. increase volume of solid part – with depth for all three sites but it is not the case in reality for the Forest and Orchard site. For these sites, the layering of the soil is not captured by the maps. This shows that uncertainty of mapped soil hydraulic properties mainly come from the uncertainty of the soil maps used as inputs to compute the soil hydraulic maps. Regarding the KS there are notable differences both in vertical change and magnitude even when measured soil properties are used to compute it. This underpins that the prediction of saturated hydraulic conductivity has high prediction uncertainty (Nasta et al., 2021b) which is due to a number of reasons: high variability of KS in space (Usowicz and Lipiec, 2021) and time (Alletto et al., 2015), the variability of KS cannot be fully explained by basic soil properties (Vereecken, 2002) and difficulty in defining the volume of measured sample that can support the description of soil hydrological processes at profile scale (Rezaei et al., 2016).

Simulation of soil moisture

According to the guidelines of Harmel et al. (2018), we considered the calibration-validation (REF model) at the Forest Site as acceptable (the two-year averaged NSME = 0.50). Soil water content was under- and overestimated in wetter and drier periods respectively. Apart from this, the REF model simulated the effects of snow melt, precipitation and evapotranspiration realistically, with residuals moving in an acceptable range.

Table 3. Performance of soil hydraulic maps computed for the Balaton catchment based on the measured profile data of the Hungarian Detailed Soil Hydro-physical Dataset. KS: saturated hydraulic conductivity, MRC: soil moisture retention curve, ME: mean error, RMSE: root mean square error, N: number of samples/number of theta-h pairs.

Soil hydraulic map	Depth	$\log_{10}$KS			MRC		
		ME	RMSE	N	ME	RMSE	N
	cm	$\log_{10}$ (cm day^{-1})		–	cm^3 cm^{-3}		–
HUN-MAP_EU-PTF	0–30	–0.36	1.06	37	0.003	0.069	1694
	30–60	0.09	0.81	36	0.005	0.071	1674
	60–90	0.09	0.86	35	0.011	0.073	1632
EU-SHG	0–2.5	–0.17	1.58	37	–0.024	0.078	1727
	2.5–10	–0.39	1.48	37	–0.008	0.074	1727
	10–22.5	–0.40	1.06	37	0.007	0.071	1723
	22.5–45	–0.09	0.62	37	0.015	0.070	1718
	45–80	0.62	1.32	36	0.025	0.077	1696
	80–150	0.31	0.85	34	0.029	0.080	1555
	150–200	0.08	0.89	14	0.038	0.093	427

Model efficiency of the calibration and validation periods differed notably, which suggests that longer simulation period will improve model performance.

Parameter fitting was burdened with data uncertainty: based on visual evaluation (Dorigo et al., 2013), the soil moisture data from the 10 cm sensor had to be excluded from the analysis. This is an unfavourable factor for the parameter fitting process, as this sensor monitored the critical topsoil layer of the soil column, where the water content variations are the most sensitive for meteorological conditions. The absence of locally measured precipitation also meant a source of error as the water budget calculations showed significant sensitivity to the atmospheric boundary time series. Notable overestimations (0.1–0.2 cm^3 cm^{-3} in the spring of 2017, Figure A11) were present for the REF variant, which could not be eliminated with parameter adjustment. This indicates that the applied boundary conditions were biased. To overcome this issue, a new precipitation gauge was installed at the Forest Site, which will help improving model accuracy in the future. The goodness of fit of the other four model variants were not acceptable, the NSME was negative in four cases. The mean coefficients of determination between the measured and simulated soil water content values were between 0.48 and 0.79 for the site. The lower values were obtained for 100 cm soil depth.

At the Orchard Site the variability of soil water content was the lowest among the three sites, which is partly the result of the lowest amount of precipitation in the studied period. Only the calibrated model provided acceptable results for soil moisture (NSME = 0.54), while variants with mapped soil hydraulic properties (HUN-MAP_EU-PTF, EU-SHG) yielded negative NSME values (Table 4). Underestimation of soil moisture time series occurred in wet periods, while over-prediction was not characteristic. The highest prediction error occurred in the wettest period of the simulation, as a result of a major precipitation event (09-2018). Nor the calibrated, neither any other model variants were able to reproduce the sharp appearance of the wetting front in the deepest (95 cm) layer. This suggests the presence of preferential flow paths or other sources of strong non-linear behaviour (e.g MRC hysteresis), which allow the quick advance of the wetting front. However, as most soil hydraulic databases provide only the single-porosity Mualem-van Genuchten parameters, we also considered single-porosity matrix flow. It is noteworthy that the effect of initial conditions disappeared after only 3 months, and later on the five variants led to similar soil moisture time series with major differences appearing only after large precipitation events.

The mean coefficients of determination between the observed and simulated time series with predicted soil hydraulic properties for the site were between 0.55 and 0.86. Lower values (0.35–0.62) were obtained at 95 cm soil depth, which can be attributed to the underestimation of the only major soil moisture peak.

Soil moisture simulations proved to be the most accurate at the Grassland Site, where all five model variants resulted in positive NSME values. Furthermore, according to Harmel et al. (2018) the REF model results turned out to be excellent (Figure 2, Table 4). Calculations represented real world processes reliably: soil moisture varied intensively in the topmost layer indicating strong dependence from atmospheric conditions. This significant temporal variation showed a rapid decrease with depth: the ranges of measured/simulated water content at 20 and 40 cm are only half of the range at 10 cm. This is in line with the observed characteristics of the soil profile: the generally high clay content is accompanied by relatively high organic matter content in the topsoil (the highest OM content among the three studied sites), which rapidly drops with depth. Measured, database derived and calibrated vertical profiles of the saturated water content and hydraulic conductivity also suggest such a hydraulic behaviour (Figure A3). All model variants over-predicted measured values, when the soil started to dry out and through dry periods. Under-prediction is characteristic when the water content of the soil is close to saturation. At 10 cm depth, MEAS_SHP and MEAS_EU-PTF usually overestimated, while in contrast HUN-MAP_EU-PTF and EU-SHG under-predicted the soil water content in most of the studied period. Except in the case of MEAS_SHP, at 20 cm depths mainly under-prediction occurred with all model variants. At 40 cm depth all model variant underestimated the soil moisture time series.

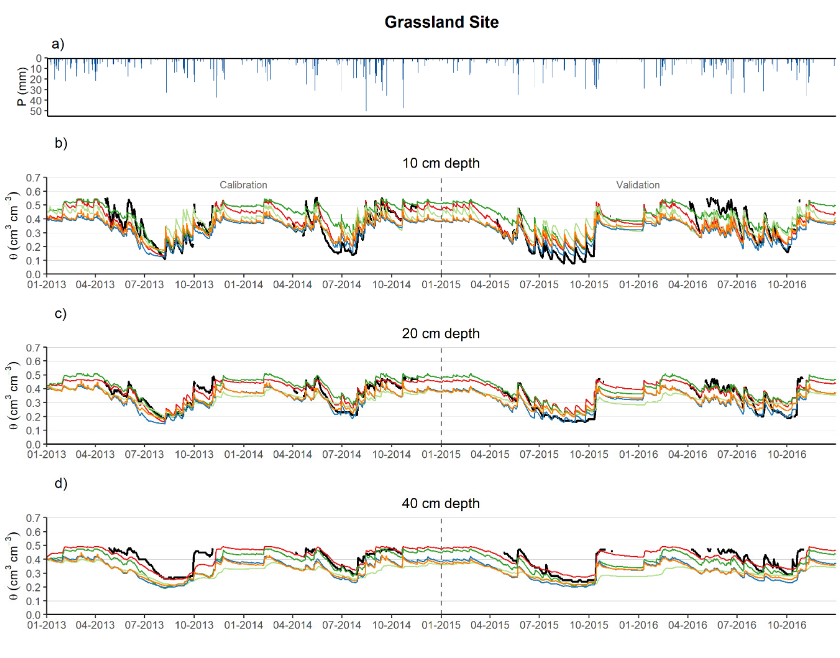


Fig. 2. Precipitation (a), measured and simulated soil moisture time series at the Grassland Site for depths 10 cm (b), 20 cm (c) and 40 cm. Blank measured data indicate periods of low soil temperature, where measurements are not reliable.

Table 4. Outcomes for model efficiency of soil moisture simulations with the five model variants, the number of measured soil moisture data per layer and the calibration-validation periods. Overall database reliability rank Dimension: NSME [–], RMSE [cm^3 cm^{-3}], ME [cm^3 cm^{-3}], R^2 [–].

Name of the site	Goodness-of-fit by model variants	REF	MEAS_SHP	MEAS_EU-PTF	HUN-MAP_EU-PTF	EU-SHG	Number of measured soil water content per soil layer	Calibration period	Validation period
Forest Site	NSME	0.50	–0.80	–0.52	–0.47	–0.65	568	01/01/2016–31/12/2016	01/01/2017–31/12/2017
	RMSE	0.04	0.076	0.075	0.075	0.078			
	ME	0.03	0.06	0.07	0.06	0.07			
	R^2	0.79	0.48	0.56	0.62	0.55			
Orchard Site	NSME	0.54	0.15	0.07	–1.81	–0.69	391–478	01/02/2018–31/12/2018	01/01/2019–31/07/2019
	RMSE	0.02	0.024	0.024	0.041	0.032			
	ME	0.01	0.02	0.02	0.03	0.03			
	R^2	0.86	0.74	0.79	0.55	0.70			
Grassland Site	NSME	0.71	0.49	0.19	0.28	0.34	760–817	01/01/2013–31/12/2014	01/01/2015–31/12/2016
	RMSE	0.05	0.07	0.09	0.09	0.08			
	ME	0.04	0.06	0.08	0.08	0.07			
	R^2	0.87	0.85	0.79	0.88	0.85			
Overall rank: soil moisture	NSME	1	2	3	5	5	Performance ranked with respect to model efficiencies combined for the three Sites: 1 – best; 5 – worst		
	RMSE	1	2	4	4	5			
	ME	1	2	4	4	4			
	R^2	1	5	3	2	4			
Overall rank: water budget		Ref	2	4	1	3	Performance ranked according to water budget accuracy, combined for the three Sites: 1 – best; 4 – worst		

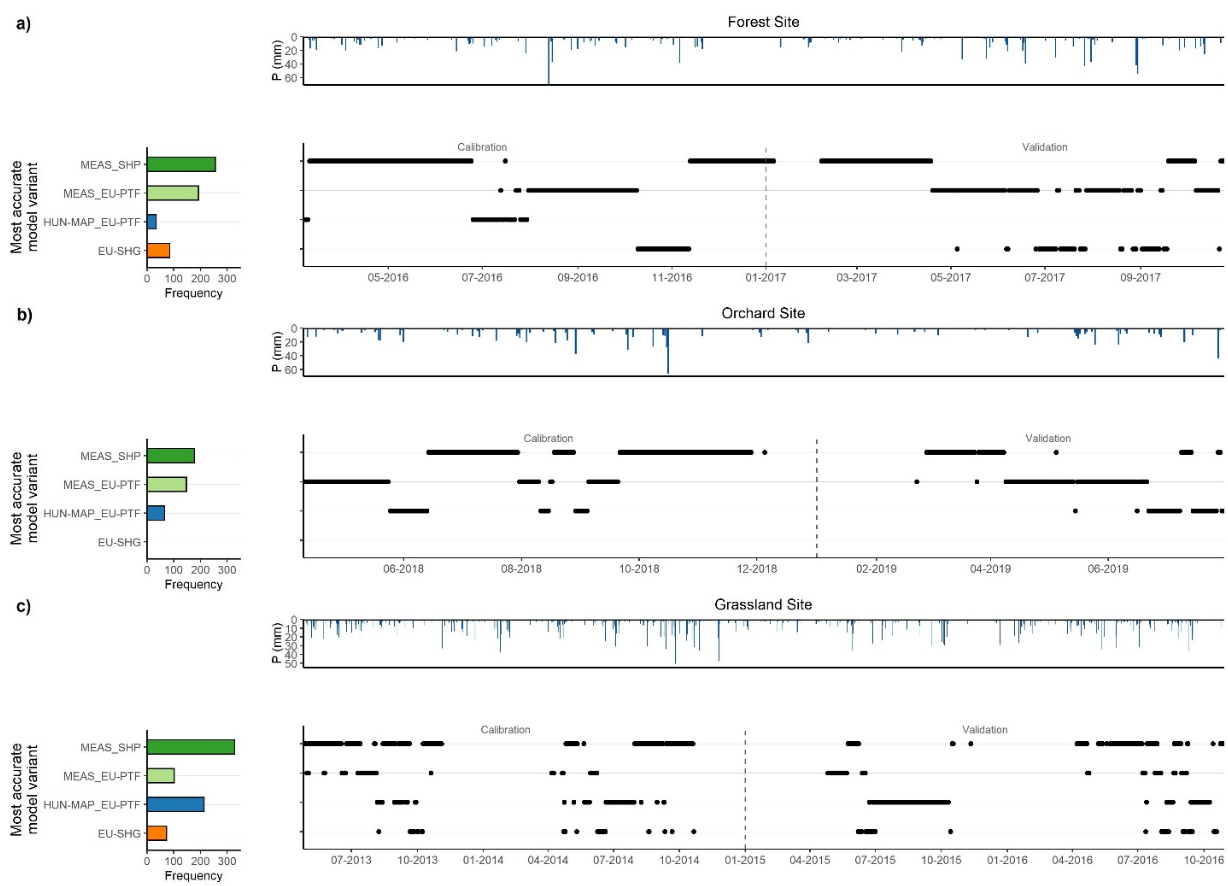


Fig. 3. The most accurate model variants based on mean absolute error of the simulated soil water content, computed by day for the whole soil profile in the a) Forest, b) Orchard and c) Grassland sites.

As expected, the calibrated soil parameters led to the best model performance at all locations, not only for the Nash-Sutcliffe efficiency (NSME was 0.50, 0.54 and 0.71 for the Forest, Orchard and Grassland Site respectively), but also performed best for any other efficiency metrics. The other four variants had different orders from site to site, but when considering the overall rank (for all three sites) the simulations based directly on the measured soil hydraulic parameters (MEAS_SHP) provided second best agreement. The combination of in situ measured primary soil properties and the EU_PTFs ranked third. The two variants based solely on soil maps performed the weakest, yielding negative NSME values for two sites (Table 4).

Beside the common model efficiency measures, we also compared the accuracy of the model variants on a daily basis, using mean absolute error of the simulated soil moisture values at all depths (the REF variant was not included in this analysis to allow a more detailed comparison of the four database derived model set ups) (Figure 3).

For all studied sites the MEAS_SHP model variant had the lowest mean absolute error for most of the studied period. For the Forest and Orchard Site the MEAS_EU-PTF model variant provided the second most accurate simulation; if only validation period was considered, MEAS_EU-PTF outperformed the MEAS_SHP. When soil parameters were derived from soil hydraulic maps, the one using national soil information (HUN-MAP_EU-PTF) resulted more accurate soil moisture simulations, than the European (EU-SHG) in the case of Orchard and Grassland sites (Figure 3). Interestingly, for the Forest Site, the EU-SHG model variant was more accurate than the HUN-MAP_EU-PTF, which might be due to the lower predictive power of the REF model compared to the other two sites.

Water budget comparison

Major differences occurred in the simulated water budgets of the REF variants among the three sites, which can be attributed to the different governing environmental conditions and thus varying atmospheric fluxes (Table 5).

At the Forest Site the annual average precipitation sum exceeded PET and had a notable, 20% simulated interception. Most of the throughfall infiltrated, providing enough water to increase soil water storage (with 88 mm per year) beside of covering 93% of the PET. In line with the large evapotranspirative capacity of the forest canopy, ET dominated the output side of the water balance. Due to this dominance of actual ET, the amount of runoff was almost negligible (0.6%). No percolation occurred, indicating that the infiltrated water remained in the upper ~100 cm domain. This is supported by the fact that the soil moisture sensor at 100 cm depth registered only an almost negligible soil water content change throughout the two years (Figure A11). The PET exceeded precipitation sum only at the Orchard Site with more than 200 mm per year, indicating much drier climatic conditions at this location. However, due to the lower precipitation sum, the loose vegetation cover and the applied low LAI time series (Figure A8), simulated actual ET turned out to be the lowest. As a result of the minimal interception and the low ET/PET ratio, the REF variant yielded 5.4% soil water storage increase and 10.4% percolation as well. The latter can be attributed to one single heavy rainfall event, the only time, when soil water content showed a positive change and increased above field capacity at 95 cm (deepest measurement). PET was the lowest at the Grassland Site, 90% of it was covered by actual ET. This was possible due to the sufficient amount of rainfall and on the expense of 11% storage decrease. At this location percolation was a significant component of the water budget (21% of precipitation). As expected, runoff was the highest here both in absolute and relative sense (68 mm year^{-1} and 8%) out of the three sites.

At each site, the four model variants resulted in minor to moderate water budget differences compared to the reference runs (REF variants). These differences are only partially in line with the model efficiency indicators: the model reliability (overall rank) judged by (i) the accuracy of the simulated soil moisture time series and by (ii) the water budget leads to a different order of model variants (Table 4). At the Forest Site, the on-site measured soil hydraulic parameters (MEAS_SHP) resulted in increased runoff (8.4% of total precipitation), while the positive storage change and actual ET was both reduced. On the other hand, the three model variants with weaker soil moisture overall rank led to similar water budgets as the REF with only slight differences (–2% to 5%) in storage change and ET. Especially the EU_SHG version approximated closely the reference variant. Water balances differed in actual ET, percolation and storage change at the Orchard Site. Only the HUN-MAP_EU-PTF variant reproduced the positive storage change indicated by the REF, and neither of the four variants could approximate the volume of percolation. At the Grassland Site major differences occurred in soil water storage, runoff and percolation. Runoff estimates ranged from zero (EU_SHG) to more than three times the REF value (MEAS_EU-PTF). Here, the MEAS_SHP provided the best match with the reference variant water budget.

DISCUSSION

Soil hydraulic maps

The uncertainty of mapped soil hydraulic properties can originate from two sources: the soil maps used as input soil data for the predictions and the PTFs applied to compute the soil hydraulic properties (Dai et al., 2013; Van Looy et al., 2017). As expected, the predictions based on the national soil maps (HUN-MAP_EU-PTF) are more accurate than the one based on the global soil map (EU_SHG). Further improvement in the performance of the soil hydraulic maps could be gained by using national soil maps based on a higher soil profile density with more detailed vertical information as input and application of PTF derived on local soil hydraulic dataset.

Table 5. Average annual precipitation, interception and potential evapotranspiration at the Sites.

Name of the site	Annual average fluxes		
	Precipitation	Interception	Potential evapotranspiration
	mm year^{-1}		
Forest Site	794	158	750
Orchard Site	701	30	912
Grassland Site	797	101	639

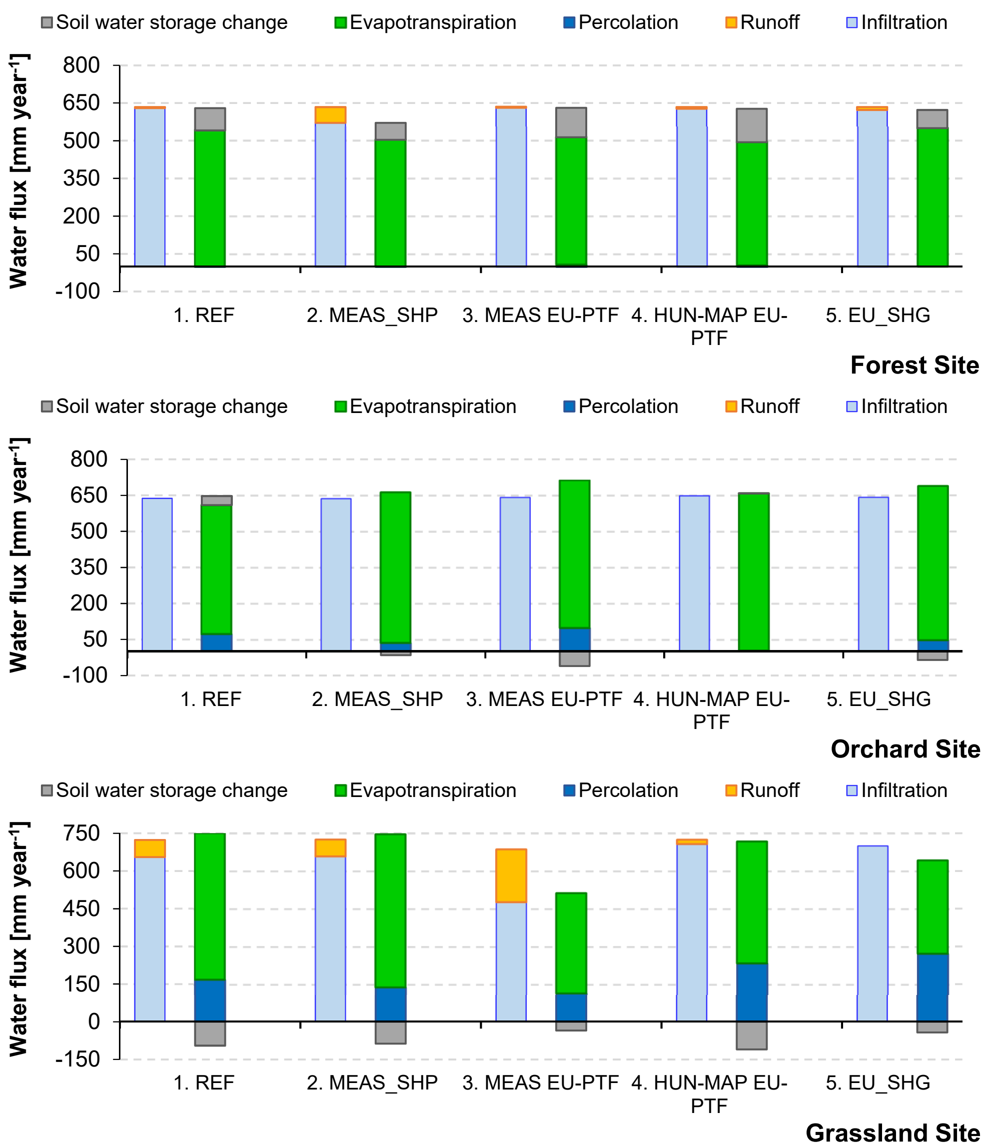


Fig. 4. Average annual water budget for the five model variants at the Forest, Orchard and Grassland Sites. First columns indicate the fate of precipitation at the soil surface; Second columns show hydrological processes in the modelled soil domains (evapotranspiration and root water uptake, recharge and change in soil water storage); For better clarity, water intercepted and evaporated at vegetation surface is not displayed.

Site specific lessons

Regarding both the sites and the model variants, soil moisture and water budget simulation results showed a remarkable variation. This is in line with changes in local environmental conditions (meteorology, vegetation and soil) as well as with differences in the measurement/database derived soil profiles. The vertical distribution of water retention characteristics and especially KS showed major differences for the five model variants at each site (Figure A5–7). Beside the depth distribution of MRC and HCC parameters, the position of soil layers also contributed to the observed differences of the results, as the numerical simulation is rather sensitive to this input. This highlights the importance of vertical discretization, which might be uncertain in soil datasets. For instance, if a textural change occurs between 70 and 90 cm soil depth it might not be captured due to the standardized layering – i.e., 0–5, 5–15, 15–30, 30–60, 60–100, 100–200 cm – of the soil map.

At the Forest site both the field and laboratory measurements of hydraulic conductivity were burdened with various complications (extensive root network near the soil surface, slow/incomplete saturation of the samples, etc.), which led to data uncertainty. Especially soil hydraulic characteristics showed great variability that can influence local data collection and modeling. The hydrological effects of this inherent variability in the MRC and KS are strongly scale-dependent and are probably the most defining at the plot-hillslope scale (Baveye and Laba, 2015). At certain depths, hydraulic conductivity values from calibration (REF), measurements (MEAS_SHP) or derived by PTFs differed with orders of magnitude. Such data uncertainty is a general experience for PTF derived KS data at local, regional and global scales (Gupta et al., 2022; Nasta et al., 2021b; Zhang et al., 2018). This originates from the (i) lack of standardized KS measurement methods and (ii) limited spatial and temporal information about environmental conditions, which influence KS, e.g., porosity governed by biological and human activity. These limit the efficiency of KS PTFs predictions in general. The strong water content dependency of to the HCC and the frequent absence of k(h) measurements (as in case of this study as well) further increases data uncertainty associated to field- and/or map-based hydraulic conductivity data (De Pue et al., 2019). As one of the most sensitive parameters of soil moisture simulations is the hydraulic conductivity (De Pue et al., 2019), its uncertain vertical distribution explains the weak model performance (negative NSME for all variants expect for REF) at the Forest site. Furthermore, hydraulic conductivity has a defining role also on water budget results: runoff, percolation and storage change responded sensitively to alterations in HCC profiles. This outcome was relevant not only at the Forest but at all three sites.

Simulated storage change and percolation responded sensitively at the Orchard and Grassland Sites for the variation of soil hydraulic parameters: at the Orchard, the increased downward flux decreased the volume of stored soil water or vice versa. Modelled percolation varied between 0 and 98 mm year^{-1}. At the Grassland Site, percolation ranged between 115 and 272 mm year^{-1} and beside storage, it influenced actual ET and runoff. These ranges show a major uncertainty in the estimation of groundwater recharge. In case of a distributed parameter hydrological model application such local uncertainties would accumulate along the flow paths, leading to an increased over/underestimation of other percolation-dependent water budget components (baseflow and discharge), as well.

At the Grassland Site water budget results raised an interesting issue, all variants resulted in relatively high values of percolation, an outcome that contradicts our a priori expectations considering the high clay content at this site. One explanation for this phenomenon is the possible presence of preferential flow paths, which is supported by simulation and field experience. At 40 cm depth the measured soil water content changes slowly and in a smooth manner except for two moderate rainfall events, which induced unexpectedly sharp increases in the observed water content. Simulations could not reproduce this strongly non-linear response. During the field survey we observed the presence of pseudo-gleyic expansive clay in the soil profile, which might offer a possible explanation for the irregular soil moisture behavior. Such expansive soils tend to have special shapes of the MRC and HCC due to the dis- and reappearance of fissures during the swelling-shrinking process (Ito and Azam, 2020). Another possible cause for the observed non-linear change can be the presence of occasional interflow, a phenomenon possibly occurring in this region, however neglected by the applied Hydrus-1D algorithm. Either its preferential flow paths and/or interflow, this experience underlines the limited capacity of available soil hydrological databases to represent such complex behavior by using the most common single-porosity soil hydraulic model. Incorporating dual-porosity information into PTF development is a promising research direction to cope with this issue (Zhang et al., 2022).

General experience

Beside the differences, there were some similarities between the three sites, as well. In line with expectations and common sense, the simulations based directly on the measured soil hydraulic parameters (MEAS_SHP) provided second best agreement with observed soil moisture data, while PTF estimates based on measured primary soil properties (MEAS_EU-PTF) ranked as third, and the soil hydraulic parameters derived from maps ranked the weakest. The NSME turned out to be negative for several database model variants. While the national and continental database derived results ranked the weakest with respect to soil moisture, the comparison of the water budgets interestingly led to a different outcome. The HUN-MEAS_EU-PTF turned out to provide the best approximation of the REF variant. These outcomes indicate the importance of field experience and the acceptable performance of PTF derived soil hydraulic parameters in soil water simulations if locally measured basic soil data is used as input.

The performance of the model was influenced by several local environmental factors, such as dense root network near the forest floor, temperature effects on the measured near-surface soil moisture contents, possible presence of macro-pores and/or fissures, expansive clay with non-linear behavior, which limits the accuracy of automated soil moisture simulations at soil profile and catchment level if soil input data is based solely on large-scale soil hydraulic databases.

The overall ranks for model efficiency and for the water budget results also raise questions about the local representativeness/accuracy of catchment scale, distributed parameter hydrological simulations. Even though the recent technological advances, the calibration-validation of cell-based catchment models still relies mostly on time series recorded at a relatively low number of observation points within the watershed. This calibration practice provides only a limited control over the adjustment of spatially distributed parameters. Therefore, the seemingly good model efficiencies can be the result of over-parametrization (Fatichi et al., 2016).

Two main options can offer solution for this issue, one of them is the multi-objective calibration strategy. Beside pointwise data, the multi-objective calibration relies also on spatially continuous data sources of hydrologic variables, e.g. snow cover, surface soil moisture content, evapotranspiration or temporal water coverage (Gomis-Cebolla et al., 2022; Kozma et al., 2022). Among these variables remotely sensed soil moisture data could offer the most relevant information for the adjustment of soil parameters. However, such soil moisture products haven't become very popular among modelers for a number of reasons (Tong et al., 2021). Thus, currently these products have limited and "costly" capacity to increase the spatial representativeness of hydrological simulations.

The improvement of the spatial input data quality is the other option. The increasing resolution and accuracy of the input soil data and the good discharge agreement at the gauging stations together offer the illusion of reliable spatial representation of surface and subsurface water movements and conditions. However, as this research points it out, there are significant differences between soil databases both in case of soil hydrological parametrization and vertical distribution of soil layering within the soil profile. These can lead to significantly different simulation outcomes at cell-level, leading to uncertain spatial representations of hydrological processes.

This emphasizes the importance of proper aim definition for each model study: whether an analysis primarily aims to simulate (i) soil moisture dynamics or (ii) water budget and hydrological/environmental flows. Considering catchment scale hydrological modelling, the profile based (cell-level) budgets – such as the ones presented here or e.g. Vereecken et al. (1992), Nasta et al. (2021b) – can provide useful information and insight about the functional reliability of the studied soil property databases and might help to overcome the issue of over-fitted models.

CONCLUSIONS

Soil hydraulic properties derived by PTFs from continental and national soil maps still have limited capacity to provide reliable input data for the simulations of unsaturated zone hydrology at soil profile scale. Even though the recent advances in geostatistics and remote sensing, the site-specific field scale data gathering is still necessary for profile scale hydrological simulations. If local soil survey information is available for the basic soil properties – i.e. depth of genetic soil horizons, sand, silt and clay content, organic carbon content, bulk density –, soil hydraulic properties derived from those by PTFs can provide input with acceptable accuracy for profile scale simulation. The largest challenges are to improve the vertical accuracy of soil layering and to represent quantitative information about preferential flow paths.

Funding. The research presented in the article was carried out within the framework of the Széchenyi Plan Plus program with the support of the RRF 2.3.1 21 2022 00008 project and was supported by the Hungarian National Research, Development and Innovation Office (K 119475). The research reported in this paper is part of project no. BME-NVA-02, implemented with the support provided by the Ministry of Innovation and Technology of Hungary from the National Research, Development and Innovation Fund, financed under the TKP2021 funding scheme.

REFERENCES

Alletto, L., Pot, V., Giuliano, S., Costes, M., Perdrieux, F., Justes, E., 2015. Temporal variation in soil physical properties improves the water dynamics modeling in a conventionally-tilled soil. Geoderma, 243–244, 18–28. https://doi.org/10.1016/j.geoderma.2014.12.006

Arnold, J.G., Moriasi, D.N., Gassman, P.W., Abbaspour, K.C., White, M.J. et al., 2012. SWAT: Model Use, Calibration, and Validation. Trans. ASABE, 55, 4, 1491–1508. https://doi.org/10.13031/2013.42256

Baveye, P.C., Laba, M., 2015. Moving away from the geostatistical lamppost: Why, where, and how does the spatial heterogeneity of soils matter? Ecol. Modell., 298, 24–38. https://doi.org/10.1016/j.ecolmodel.2014.03.018

Bréda, N.J.J., 2003. Ground-based measurements of leaf area index: a review of methods, instruments and current controversies. J. Exp. Bot., 54, 392, 2403–2417. https://doi.org/10.1093/jxb/erg263

Breuer, L., Eckhardt, K., Frede, H.G., 2003. Plant parameter values for models in temperate climates. Ecol. Modell., 169, 2–3, 237–293. https://doi.org/10.1016/S0304-3800(03)00274-6

Buzás, I., 1988. Talaj- és agrokémiai vizsgálati módszerkönyv 2. A talajok fizikai-kémiai és kémiai vizsgálati módszerei. (Buzás István, editor). Mezőgazdasági Kiadó, Budapest.

Buzás, I., 1993. Talaj- és agrokémiai vizsgálati módszerkönyv 1. A talaj fizikai, vízgazdálkodási és ásványtani vizsgálata (Buzás István, editor). Inda 4231 Kiadó.

Campbell Scientific, Inc., 2020. Product manual: CS616 and CS625 Water Content Reflectometers. Revision: 05/2020. https://s.campbellsci.com/documents/us/manuals/cs616.pdf

Chaney, N.W., Wood, E.F., McBratney, A.B., Hempel, J.W., Nauman, T.W. et al., 2016. POLARIS: A 30-meter probabilistic soil series map of the contiguous United States. Geoderma, 274, 54–67. https://doi.org/10.1016/j.geoderma.2016.03.025

Dai, Y., Shangguan, W., Duan, Q., Liu, B., Fu, S. et al. 2013. Development of a China dataset of soil hydraulic parameters using pedotransfer functions for land surface modeling. J. Hydrometeorol., 14, 3, 869–887. https://doi.org/10.1175/JHM-D-12-0149.1

Dai, Y., Xin, Q., Wei, N., Zhang, Y., Shangguan, W. et al. 2019. A global high-resolution data set of soil hydraulic and thermal properties for land surface modeling. J. Adv. Model. Earth Syst., 11, 9, 2996–3023. https://doi.org/10.1029/2019ms001784

De Mendiburu, F., 2017. agricolae: Statistical Procedures for Agricultural Research. R package version 1.2-8.

De Pue, J., Rezaei, M., Van Meirvenne, M., Cornelis, W.M., 2019. The relevance of measuring saturated hydraulic conductivity: Sensitivity analysis and functional evaluation. J. Hydrol. 576: 628–638. https://doi.org/10.1016/j.jhydrol.2019.06.079

Decsi, B., Ács, T., Kozma, Z., 2020. Long-term water regime studies of a degraded floating fen in Hungary. Period. Polytech. Civ. Eng., 64(4 SE-Research Article), 951–963. https://doi.org/10.3311/PPci.16352

Dorigo, W.A., Xaver, A., Vreugdenhil, M., Gruber, A., Hegyiová, A. et al. 2013. Global automated quality control of in situ soil moisture data from the International Soil Moisture Network. Vadose Zone J., 12, 3, vzj2012.0097. https://doi.org/10.2136/vzj2012.0097

Đukić, V., Erić, R., Dumbrovsky, M., Sobotkova, V., 2021. Spatio-temporal analysis of remotely sensed and hydrological model soil moisture in the small Jičinka River catchment in Czech Republic. J. Hydrol. Hydromechanics, 69, 1, 1–12. doi: https://doi.org/10.2478/johh-2020-0038.

Farkas, C., Hernádi, H., Makó, A., Máté, F., 2011. Estimating climate change effects on soil water balance elements of Hungarian calcic chernozem soils. Agrokémia és Talajt., 60, 41–56.

Fatichi, S., Vivoni, E., Ogden, F.L., Ivanov, V.Y., Mirus, B. et al. 2016. An overview of current applications, challenges, and future trends in distributed process-based models in hydrology. J. Hydrol., 537, 45–60. https://doi.org/10.1016/j.jhydrol.2016.03.026

Feddes, R.A., Kowalik, P.J., Zaradny, H., 1978. Simulation of field water use and crop yield. Centre for Agricultural Publishing and Documentation, Wageningen.

Federer, A.C., 2021. Brook90 Hydrological model. http://www.ecoshift.net/brook/brook90.htm.

Fiala, K., Blanka, V., Ladányi, Z., Szilassi, P., Benyhe, B. et al. 2014. Drought severity and its effect on agricultural production in the Hungarian-Serbian cross-border area. J. Environ. Geogr., 7, 3-4 SE-, 43–51. https://doi.org/10.2478/jengeo-2014-0011

Ganot, Y., Holtzman, R., Weisbrod, N., Nitzan, I., Katz, Y. et al. 2017. Monitoring and modeling infiltration--recharge dynamics of managed aquifer recharge with desalinated seawater. Hydrol. Earth Syst. Sci., 21, 9, 4479–4493. https://doi.org/10.5194/hess-21-4479-2017

Gomis-Cebolla, J., Garcia-Arias, A., Perpinyà-Vallès, M., Francés, F., 2022. Evaluation of Sentinel-1, SMAP and SMOS surface soil moisture products for distributed eco-hydrological modelling in Mediterranean forest basins. J. Hydrol., 608, 127569. https://doi.org/10.1016/j.jhydrol.2022.127569

Guber, A.K., Pachepsky, Y.A., van Genuchten, M.T., Simunek, J., Jacques, D. et al. 2009. Multimodel simulation of water flow in a field soil using pedotransfer functions. Vadose Zone J., 8, 1, 1–10. https://doi.org/10.2136/vzj2007.0144

Gupta, S., Papritz, A., Lehmann, P., Hengl, T., Bonetti, S. et al. 2022. Global mapping of soil water characteristics parameters – Fusing curated data with machine learning and environmental covariates. Remote Sens., 14, 8, 1947. DOI:

10.3390/rs14081947

Harmel, R.D., Baffaut, C., Douglas-Mankin, K., 2018. Review and development of ASABE Engineering Practice 621: "Guidelines for Calibrating, Validating, and Evaluating Hydrologic and Water Quality Models". Trans. ASABE, 61, 4, 1393–1401. https://doi.org/10.13031/trans.12806

Hengl, T., 2017. GSIF: Global Soil Information Facilities. R package version 0.5-4. https://CRAN.R-project.org/package=GSIF

Ito, M., Azam, S., 2020. Relation between flow through and volumetric changes in natural expansive soils. Eng. Geol., 279, 105885. https://doi.org/10.1016/j.enggeo.2020.105885

IUSS Working Group WRB, 2015. World Reference Base for Soil Resources 2014, update 2015. International soil classification system for naming soils and creating legends for soil maps. 3rd Ed. FAO, Rome (Italy).

Johnson, S.G., 2014. The NLopt nonlinear-optimization package. https://nlopt.readthedocs.io/en/latest/.

Karimi, P., Bastiaanssen, W.G.M., 2015. Spatial evapotranspiration, rainfall and land use data in water accounting – Part 1: Review of the accuracy of the remote sensing data. Hydrol. Earth Syst. Sci., 19, 1 507–532. https://doi.org/10.5194/hess-19-507-2015

Kozma, Z., Ács, T., Koncsos, L., 2014. Unsaturated zone modelling: The role of soil database classification. WIT Trans. Ecol. Environ., 185. https://doi.org/10.2495/SI140181

Kozma, Z., Jolánkai, Z., Kardos, M.K., Muzelák, B., Koncsos, L., 2022. Adaptive water management-land use practice for improving ecosystem services – a Hungarian modelling case study. Period. Polytech. Civ. Eng. 66, 1 SE-Technical Notes, 256–268. https://doi.org/10.3311/PPci.18369

Loosvelt, L., Pauwels, V.R.N., Cornelis, W.M., De Lannoy, G.J.M., Verhoest, N.E.C., 2011. Impact of soil hydraulic parameter uncertainty on soil moisture modeling. Water Resour. Res., 47, 3, 1–16. https://doi.org/10.1029/2010WR009204

Makó, A., Tóth, B., Hernádi, H., Farkas, C., Marth, P., 2010. Introduction of the Hungarian Detailed Soil Hydrophysical Database (MARTHA) and its use to test external pedotransfer functions. Agrokémia és Talajt., 59, 1, 29–38.

Mohanty, B.P., Cosh, M.H., Lakshmi, V., Montzka, C., 2017. Soil moisture remote sensing: State-of-the-science. Vadose Zone J., 16, 1. https://doi.org/10.2136/vzj2016.10.0105

Monteith, J.L., 1965. Evaporation and environment. Symp. Soc. Exp. Biol., 19, 205–234.

MSZ-08.0205:1978, 1978. Determination of physical and hydrophysical properties of soils. (A talaj fizikai és vízgazdálkodási tulajdonságainak vizsgálata).

Mualem, Y., 1976. A new model for predicting the hydraulic conductivity of unsaturated porous media. Water Resour. Res., 12, 3, 513–522.

Nash, J.E., Sutcliffe. J.V., 1970. River flow forecasting through conceptual models part I — A discussion of principles. J. Hydrol., 10, 3, 282–290. https://doi.org/10.1016/0022-1694(70)90255-6

Nasta, P., Szabó, B., Romano, N., 2021a. Evaluation of pedotransfer functions for predicting soil hydraulic properties: A voyage from regional to field scales across Europe. J. Hydrol. Reg. Stud., 37, 100903. https://doi.org/10.1016/j.ejrh.2021.100903

Nasta, P., Szabó, B., Romano, N., 2021b. Evaluation of pedotransfer functions for predicting soil hydraulic properties: A voyage from regional to field scales across Europe. J. Hydrol. Reg. Stud., 37, 100903. https://doi.org/10.1016/j.ejrh.2021.100903

Nemes, A., Schaap, M., Wösten, J., 2003. Functional evaluation of pedotransfer functions derived from different scales of data collection. Soil Sci. Soc. Am., 67, 1093–1102. https://www.soils.org/publications/sssaj/abstracts/67/4/1093 (accessed 29 April 2013).

Nimmo, J.R., 2009. Vadose Water. In: Likens, G.E. (Ed.): Encyclopedia of Inland Waters: Oxford, UK, Elsevier, Vol. 1, pp. 766–777.

Orgiazzi, A., Ballabio, C., Panagos, P., Jones, A., Fernández-Ugalde, O., 2018. LUCAS Soil, the largest expandable soil dataset for Europe: a review. Eur. J. Soil Sci., 69, 1, 140–153. https://doi.org/10.1111/ejss.12499

Pásztor, L., Laborczi, A., Takács, K., Illés, G., Szabó, J. et al. 2020. Progress in the elaboration of GSM conform DSM products and their functional utilization in Hungary. Geoderma Reg., 21, e00269. https://doi.org/10.1016/j.geodrs.2020.e00269

Poggio, L., de Sousa, L.M., Batjes, N.H., Heuvelink, G.B.M., Kempen, B. et al. 2021. SoilGrids 2.0: producing soil information for the globe with quantified spatial uncertainty. Soil, 7, 1, 217–240. https://doi.org/10.5194/soil-7-217-2021

Qu, W., Bogena, H.R., Huisman, J.A., Schmidt, M., Kunkel, R., et al. 2016. The integrated water balance and soil data set of the Rollesbroich hydrological observatory. Earth Syst. Sci. Data, 8, 2, 517–529. https://doi.org/10.5194/essd-8-517-2016

R Core Team, 2019. R: A language and environment for statistical computing. https://www.r-project.org.

Rahmati, M., Weihermüller, L., Vanderborght, J., Pachepsky, Y.A., Mao, L. et al. 2018. Development and analysis of the Soil Water Infiltration Global database. Earth Syst. Sci. Data, 10, 3, 1237–1263. https://doi.org/10.5194/essd-10-1237-2018

Rezaei, M., Seuntjens, P., Shahidi, R., Joris, I., Boënne, W. et al. 2016. The relevance of in-situ and laboratory characterization of sandy soil hydraulic properties for soil water simulations. J. Hydrol., 534, 251–265. http://dx.doi.org/10.1016/j.jhydrol.2015.12.062.

Scanlon, B.R., Christman, M., Reedy, R.C., Porro, I., Simunek, J. et al. 2002. Intercode comparisons for simulating water balance of surficial sediments in semiarid regions. Water Resour. Res., 38, 12. https://doi.org/10.1029/2001WR001233

Šimůnek, J., Šejna, M., Saito, H., Sakai, M., van Genuchten, M.T., 2013. The HYDRUS-1D Software Package for Simulating the Movement of Water, Heat, and Multiple Solutes in Variably Saturated Media, Version 4.17. 4.0. University of California Riverside, Riverside.

Skierucha, W., Wilczek, A., Walczak, R.T., 2006. Recent software improvements in moisture (TDR method), matric pressure, electrical conductivity and temperature meters of porous media. Int. Agrophysics, 20, 3, 229–235.

Soil Survey Staff Natural Resources Conservation Service United States Department of Agriculture, 2020. Web Soil Survey. Available online at https://websoilsurvey.nrcs.usda.gov/. (accessed 22 January 2020).

Tong, R., Parajka, J., Salentinig, A., Pfeil, I., Komma, J. et al. 2021. The value of ASCAT soil moisture and MODIS snow cover data for calibrating a conceptual hydrologic model. Hydrol. Earth Syst. Sci. 25, 3, 1389–1410. https://doi.org/10.5194/hess-25-1389-2021

Tóth, B., Weynants, M., Nemes, A., Makó, A., Bilas, G. et al. 2015. New generation of hydraulic pedotransfer functions for Europe. Eur. J. Soil Sci., 66, 1, 226–238. https://doi.org/10.1111/ejss.12192.

Tóth, B., Weynants, M., Pásztor, L., Hengl, T. 2017. 3D soil hydraulic database of Europe at 250 m resolution. Hydrol. Process., 31, 14, 2662–2666. https://doi.org/10.1002/hyp.11203

Trodahl, M.I., Jackson, B.M., Deslippe, J.R., Metherell, A.K.,

2017. Investigating trade-offs between water quality and agricultural productivity using the Land Utilisation and Capability Indicator (LUCI) - A New Zealand application. Ecosyst. Serv., 26, PB, 388–399. https://doi.org/10.1016/j.ecoser.2016.10
Usowicz, B., Lipiec, J., 2021. Spatial variability of saturated hydraulic conductivity and its links with other soil properties at the regional scale. Sci. Rep., 11, 1, 8293. https://doi.org/10.1038/s41598-021-86862-3
van Genuchten, M.T., 1980. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. Soil Sci. Soc. Am. J., 44, 892–898.
Van Looy, K., Bouma, J., Herbst, M., Koestel, J., Minasny, B. et al. 2017. Pedotransfer functions in earth system science: Challenges and perspectives. Rev. Geophys., 55, 4, 1199–1256. https://doi.org/10.1002/2017RG000581
Vereecken, H., 2002. Comment on the paper, "Evaluation of pedo-transfer functions for unsaturated soil hydraulic conductivity using an independent data set". Geoderma, 108, 1, 145–147. https://doi.org/10.1016/S0016-7061(02)00127-1
Vereecken, H., Diels, J., van Orshoven, J., Feyen, J., Bouma, J., 1992. Functional evaluation of pedotransfer functions for the estimation of soil hydraulic properties. Soil Sci. Soc. Am. J., 56, 1371–1379. https://doi.org/10.2136/sssaj1992.03615995005600050007x
Vereecken, H., Schnepf, A., Hopmans, J.W., Javaux, M., Or, D., et al. 2016. Modeling soil processes: Review, key challenges, and new perspectives. Vadose Zone J., 15, 5, vzj2015.09.0131. https://doi.org/10.2136/vzj2015.09.0131
Wang, Q., Adiku, S., Tenhunen, J., Granier, A., 2005. On the relationship of NDVI with leaf area index in a deciduous forest site. Remote Sens. Environ., 94, 2, 244–255. https://doi.org/10.1016/j.rse.2004.10.006
Wesseling, J.G., Elbers, J.A., Kabat, P., den Broek, B.J., 1991. SWATRE: Instructions for input. Intern. Note, Winand Star. Centre, Wageningen, Netherlands 1991.
Weynants, M., Montanarella, L., Tóth, G., Arnoldussen, A., Anaya Romero, M. et al. 2013. European HYdropedological Data Inventory (EU-HYDI). EUR – Scientific and Technical Research series, Luxembourg. ISSN 1831-9424
Zhang, Y., Schaap, M.G., Zha, Y., 2018. A high-resolution global map of soil hydraulic properties produced by a hierarchical parameterization of a physically based water retention model. Water Resour. Res., 54, 12, 9774–9790. https://doi.org/10.1029/2018WR023539
Zhang, Y., Weihermüller, L., Toth, B., Noman, M., Vereecken, H., 2022. Analyzing dual porosity in soil hydraulic properties using soil databases for pedotransfer function development. Vadose Zone J., 21, 5, e20227. https://doi.org/10.1002/vzj2.20227
Zhao, Y., Rahmati, M., Vereecken, H., Or, D., 2024. Comment on ``Are soils overrated in hydrology?'' by Gao et al. (2023). EGUsphere, 2024, 1–5. https://doi.org/10.5194/egusphere-2024-629.
Zhao, H., Zeng, Y., Lv, S., Su, Z., 2018. Analysis of soil hydraulic and thermal properties for land surface modeling over the Tibetan Plateau. Earth Syst. Sci. Data, 10, 2, 1031–1061. https://doi.org/10.5194/essd-10-1031-2018

Received 25 March 2024
Accepted 10 June 2024

APPENDIX A

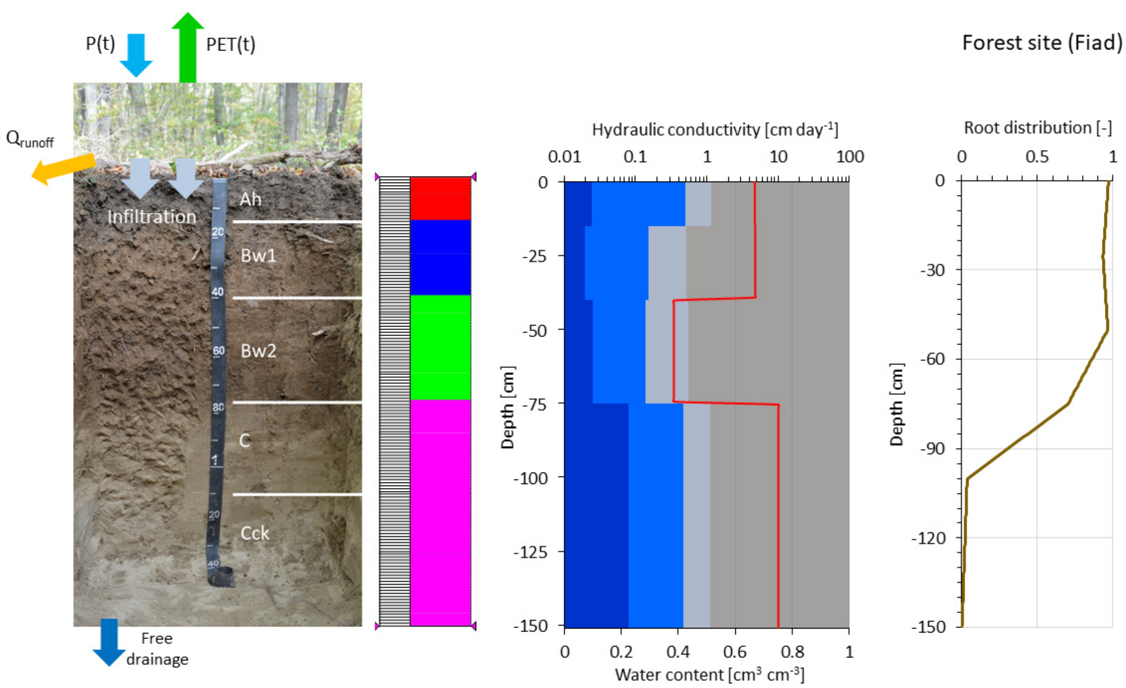


Fig. A1. Soil profile representation in the Hydrus model for the measured soil properties (MEAS_SHP) at the Forest Site: profile discretization, position of soil horizons, depth distribution of soil hydraulic properties and root distribution.

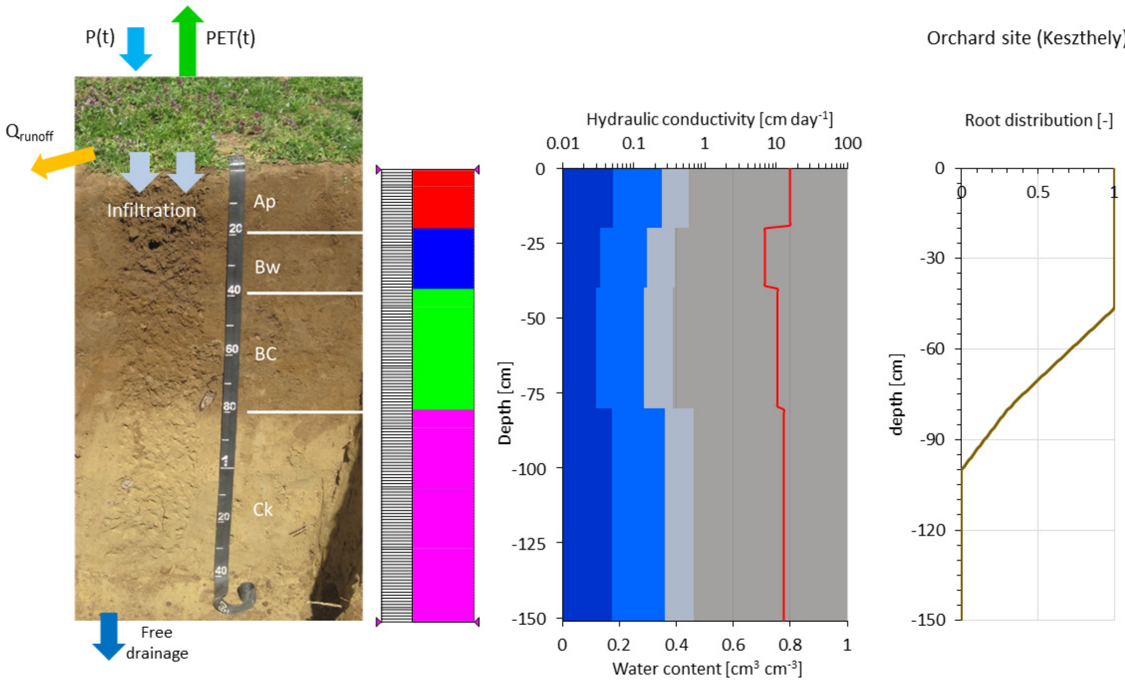


Fig. A2. Soil profile representation in the Hydrus model for the measured soil properties (MEAS_SHP) at the Orchard Site: profile discretization, position of soil horizons, depth distribution of soil hydraulic properties and root distribution.

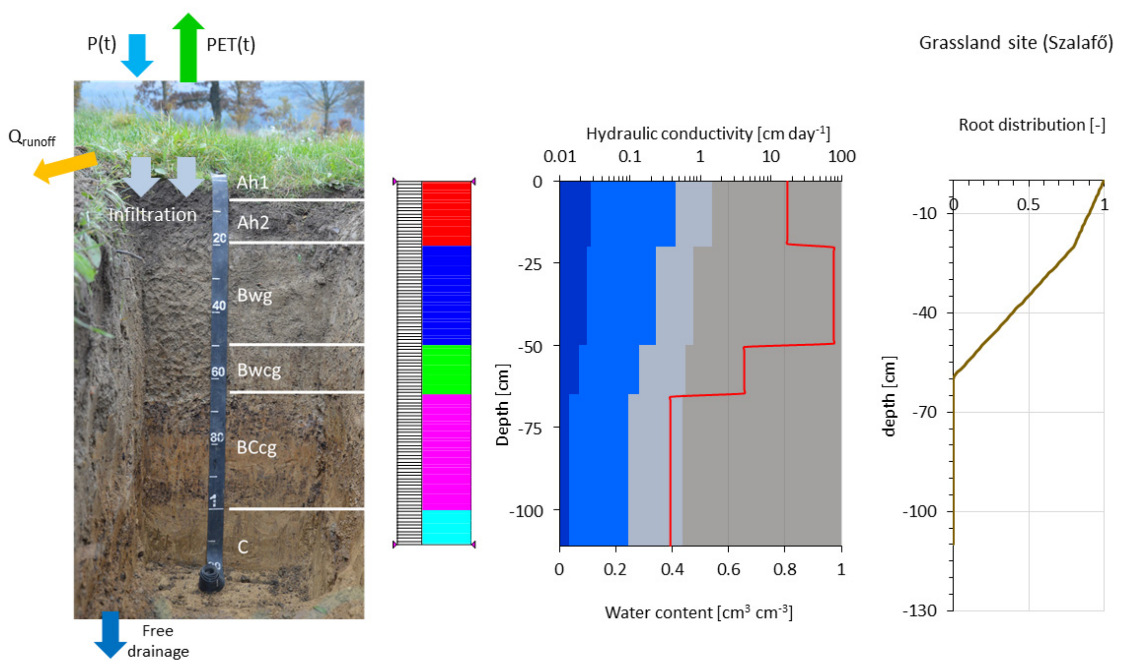
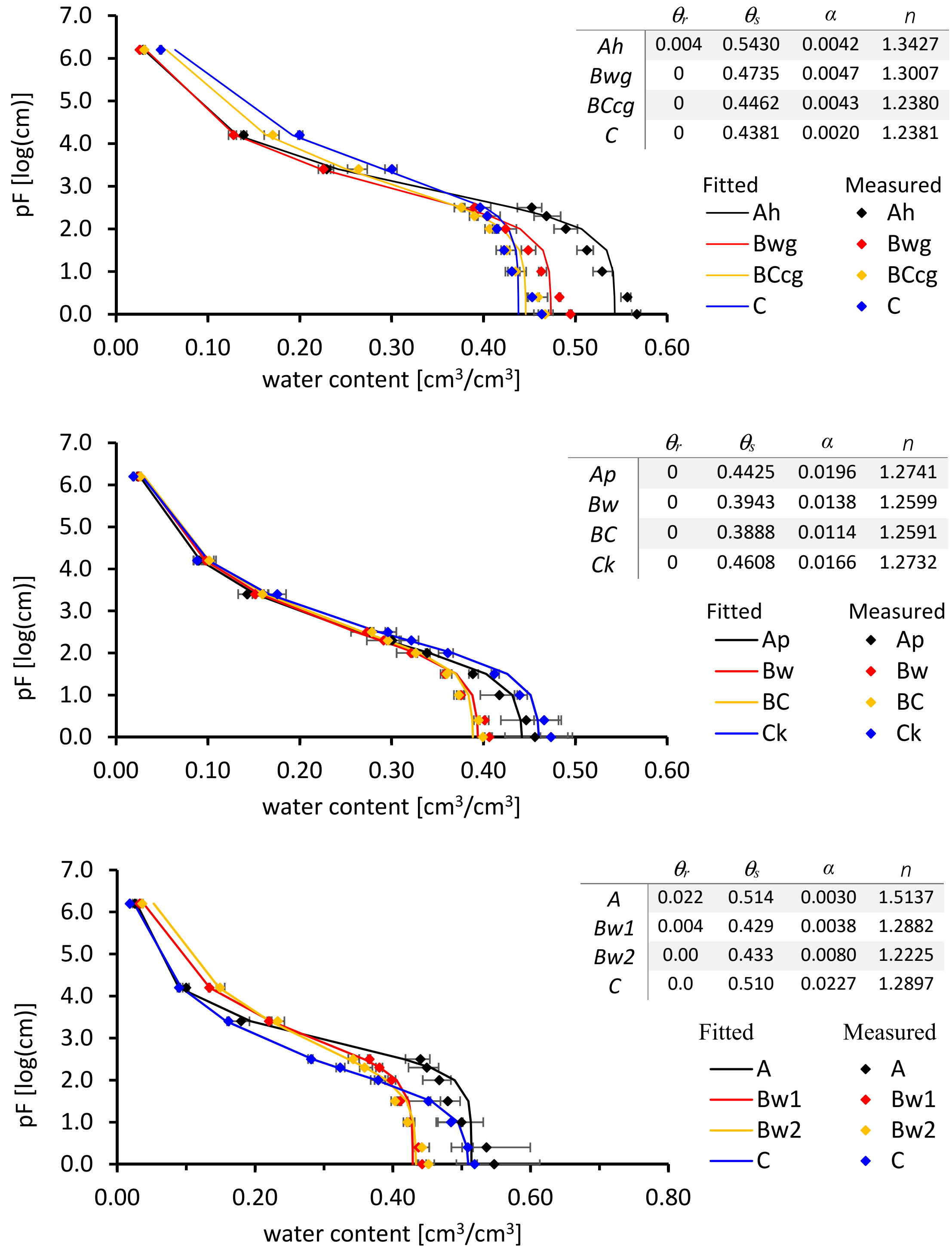


Fig. A3. Soil profile representation in the Hydrus model for the measured soil properties (MEAS_SHP) at the Grassland Site: profile discretization, position of soil horizons, depth distribution of soil hydraulic properties and root distribution.



	θ_r	θ_s	α	n
Ah	0.004	0.5430	0.0042	1.3427
Bwg	0	0.4735	0.0047	1.3007
BCcg	0	0.4462	0.0043	1.2380
C	0	0.4381	0.0020	1.2381

	θ_r	θ_s	α	n
Ap	0	0.4425	0.0196	1.2741
Bw	0	0.3943	0.0138	1.2599
BC	0	0.3888	0.0114	1.2591
Ck	0	0.4608	0.0166	1.2732

	θ_r	θ_s	α	n
A	0.022	0.514	0.0030	1.5137
Bw1	0.004	0.429	0.0038	1.2882
Bw2	0.00	0.433	0.0080	1.2225
C	0.0	0.510	0.0227	1.2897

Fig. A4. measured pF-water content values (markers) and fitted pF curves (lines) of the three study sites: Forest (top), Orchard (middle) and Grassland (bottom). Error bars indicate the range of measured water content values from the three samples taken from each soil horizon.

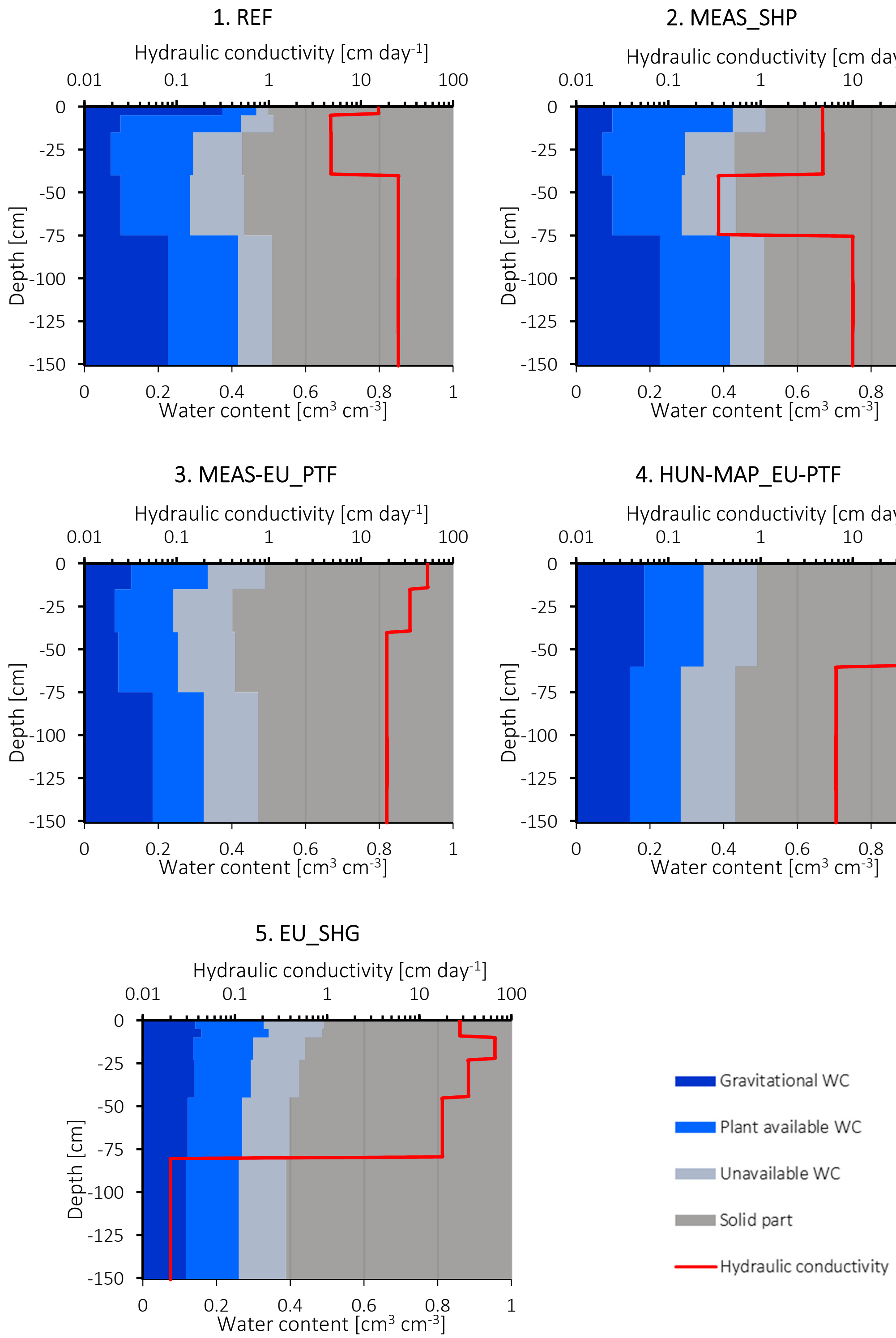


Fig. A5. Depth distribution of soil hydraulic properties for the five model variants at the Forest Site: gravitational, plant available and unavailable water contents (WC) and saturated hydraulic conductivity.

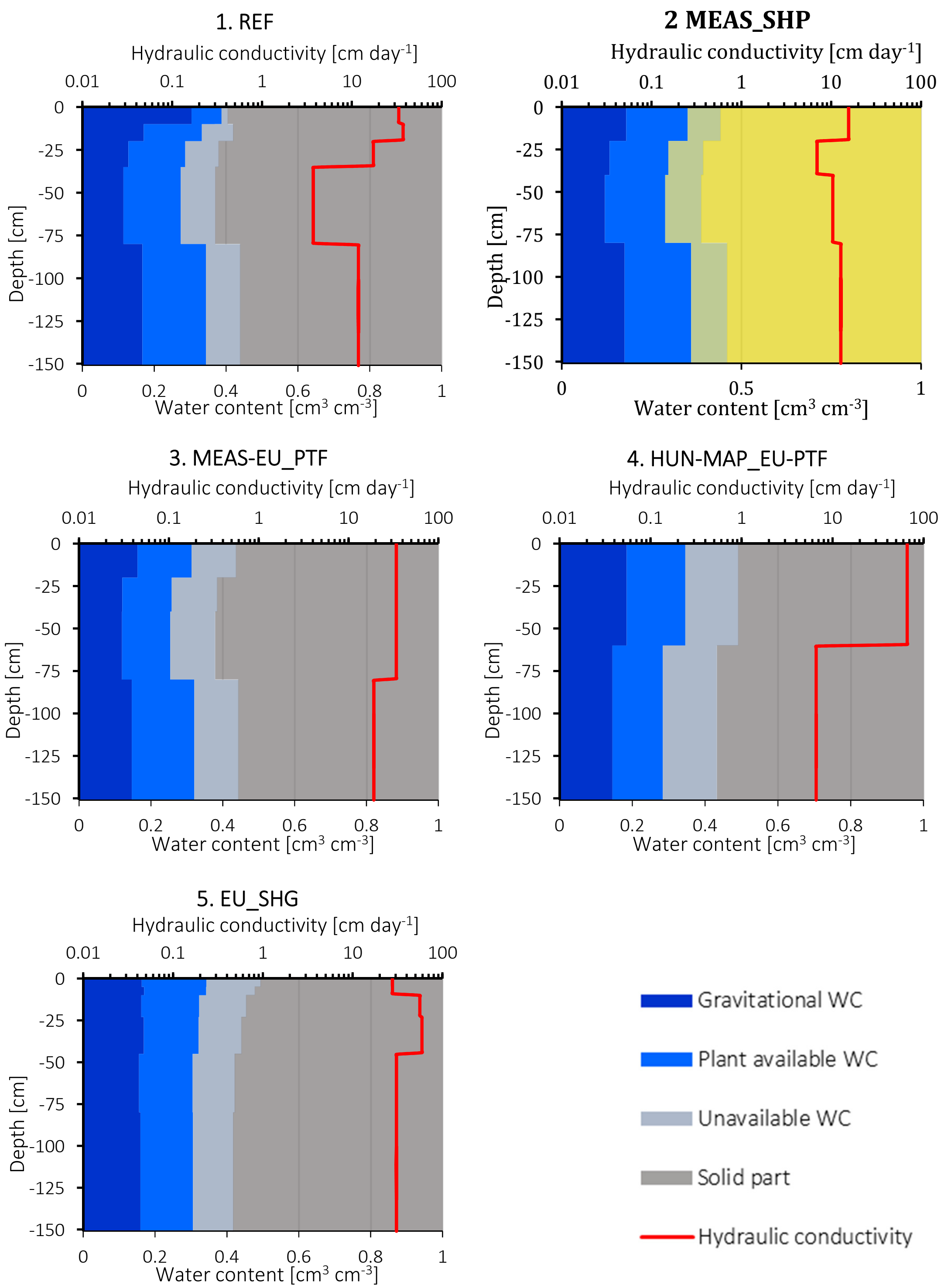


Fig. A6. Depth distribution of soil hydraulic properties for the five model variants at the Orchard Site: gravitational, plant available and unavailable water contents (WC) and saturated hydraulic conductivity.

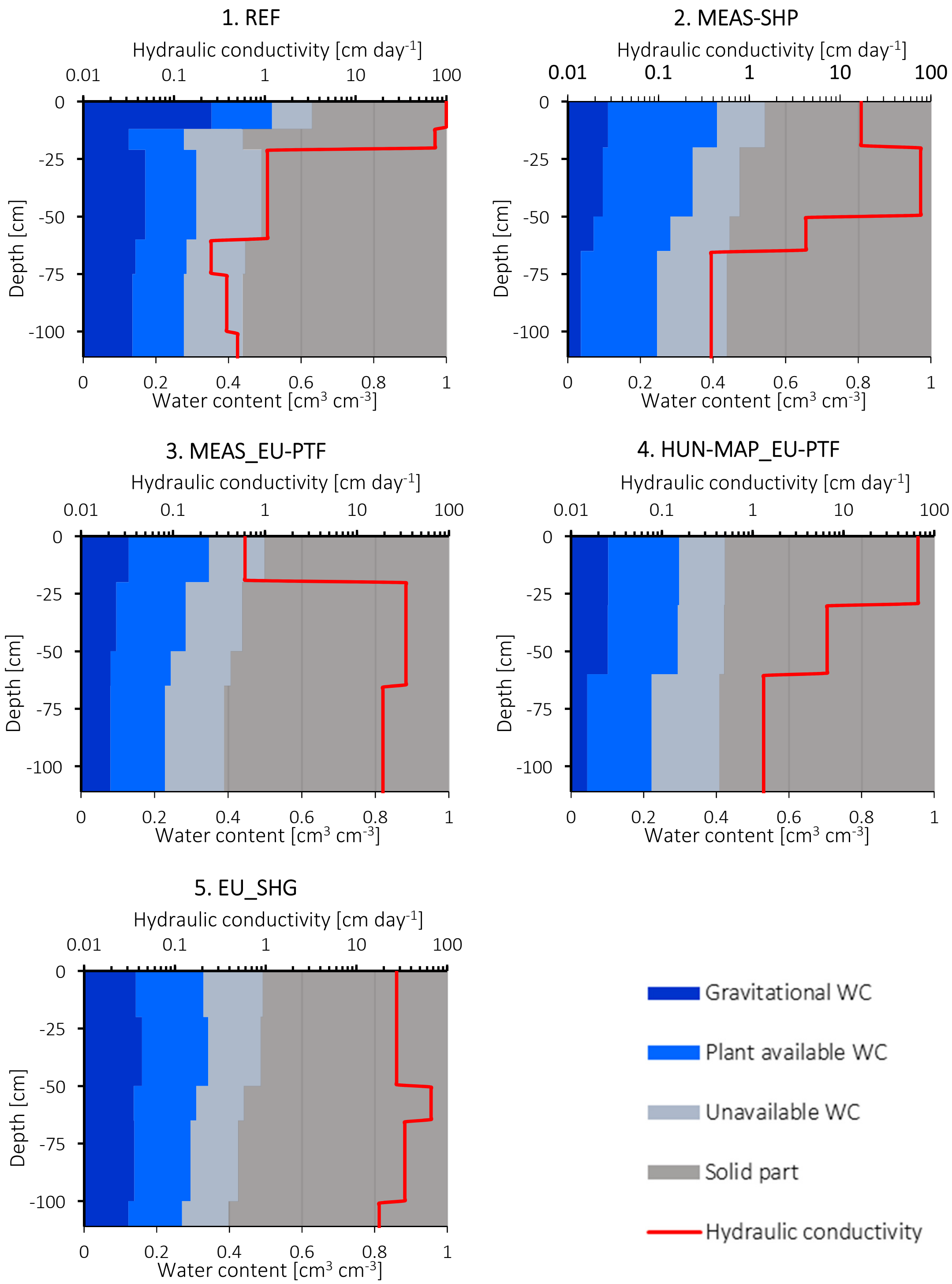


Fig. A7. Depth distribution of soil hydraulic properties for the five model variants at the Grassland Site: gravitational, plant available and unavailable water contents (WC) and saturated hydraulic conductivity.

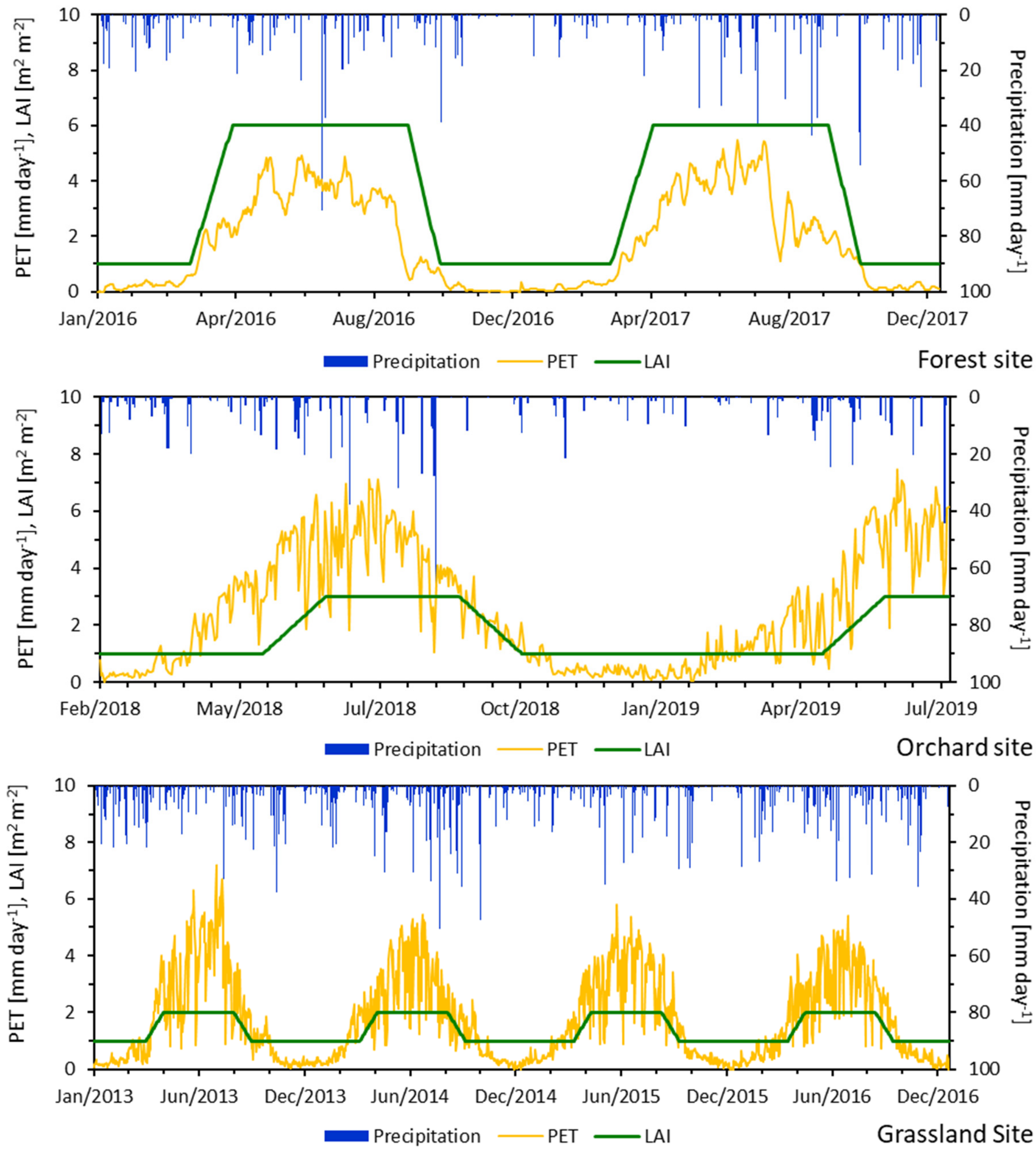


Fig. A8. Meteorological time series applied as boundary conditions at a) Forest (Fiad), b) Orchard (Keszthely) and c) Grassland (Szalafő) Site.

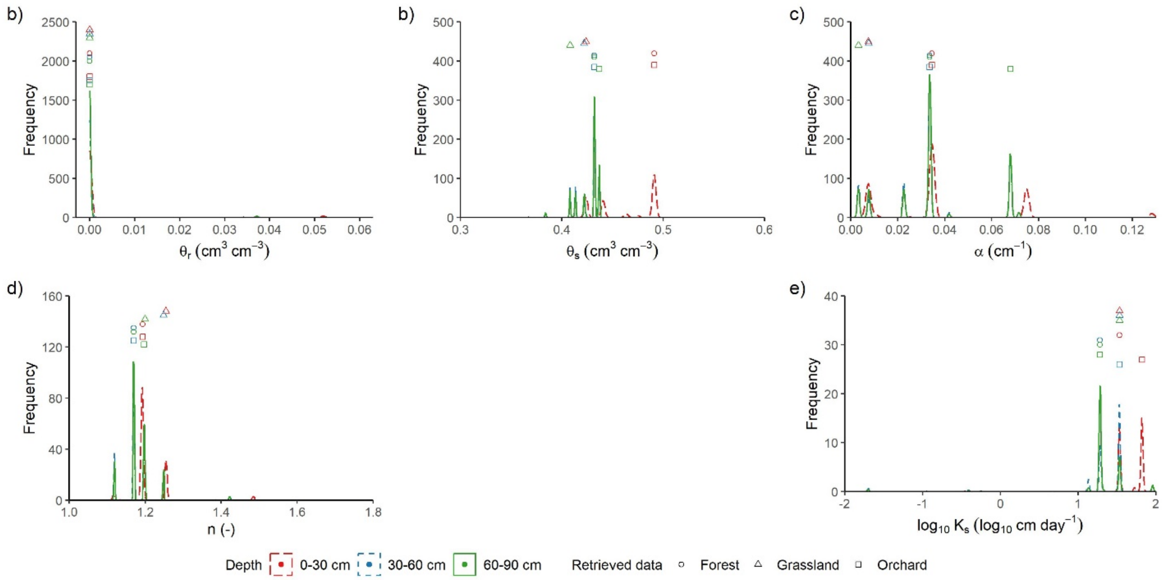


Fig. A9. Density plots of a)-d) mapped van Genuchten model parameters to describe the soil moisture retention curve and e) saturated hydraulic conductivity for the area of Balaton catchment by soil depths. Maps were derived by applying class EU-PTFs on the soil map information of the DOSoReMI.hu (HUN-MAP_EU-PTF). θ_r: residual water content; θ_s: saturated water content; α and n: fitting parameters; KS: saturated hydraulic conductivity. The van Genuchten parameters and hydraulic conductivity values retrieved from the map for the three studied sites are indicated by dot, triangle and square.

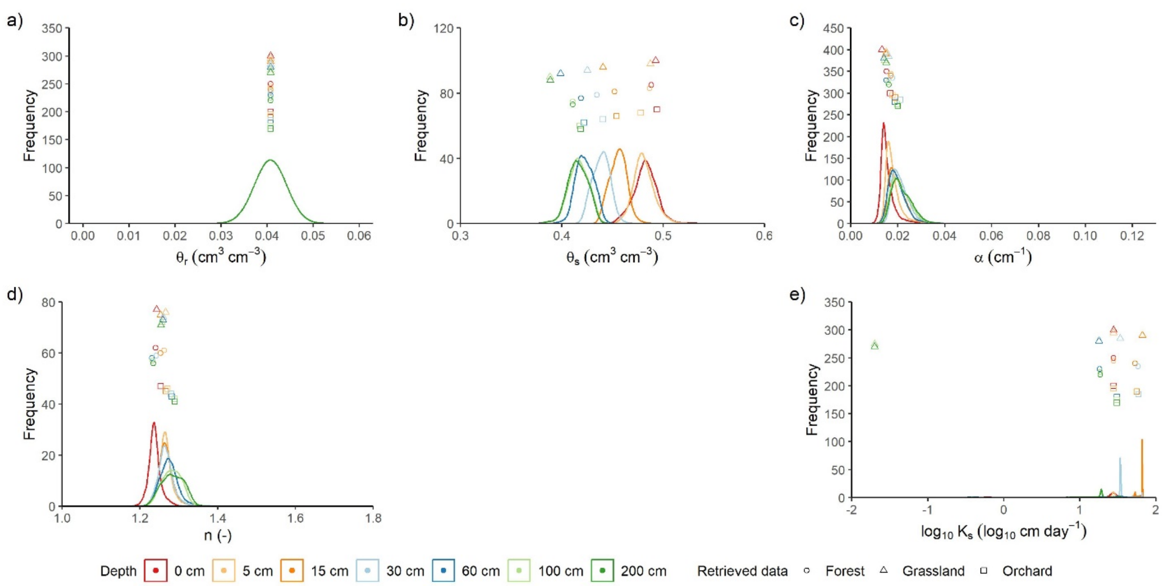


Fig. A10. Density plot of a)-d) the van Genuchten model parameters to describe the soil moisture retention curve and e) saturated hydraulic conductivity for the area of Balaton catchment by depth from the EU-SoilHydroGrids dataset (EU-SHG). θ_r: residual water content; θ_s: saturated water content; α and n: fitting parameters; KS: saturated hydraulic conductivity. The van Genuchten parameters and hydraulic conductivity values retrieved from the map for the three studied sites are indicated by dot, triangle and square.

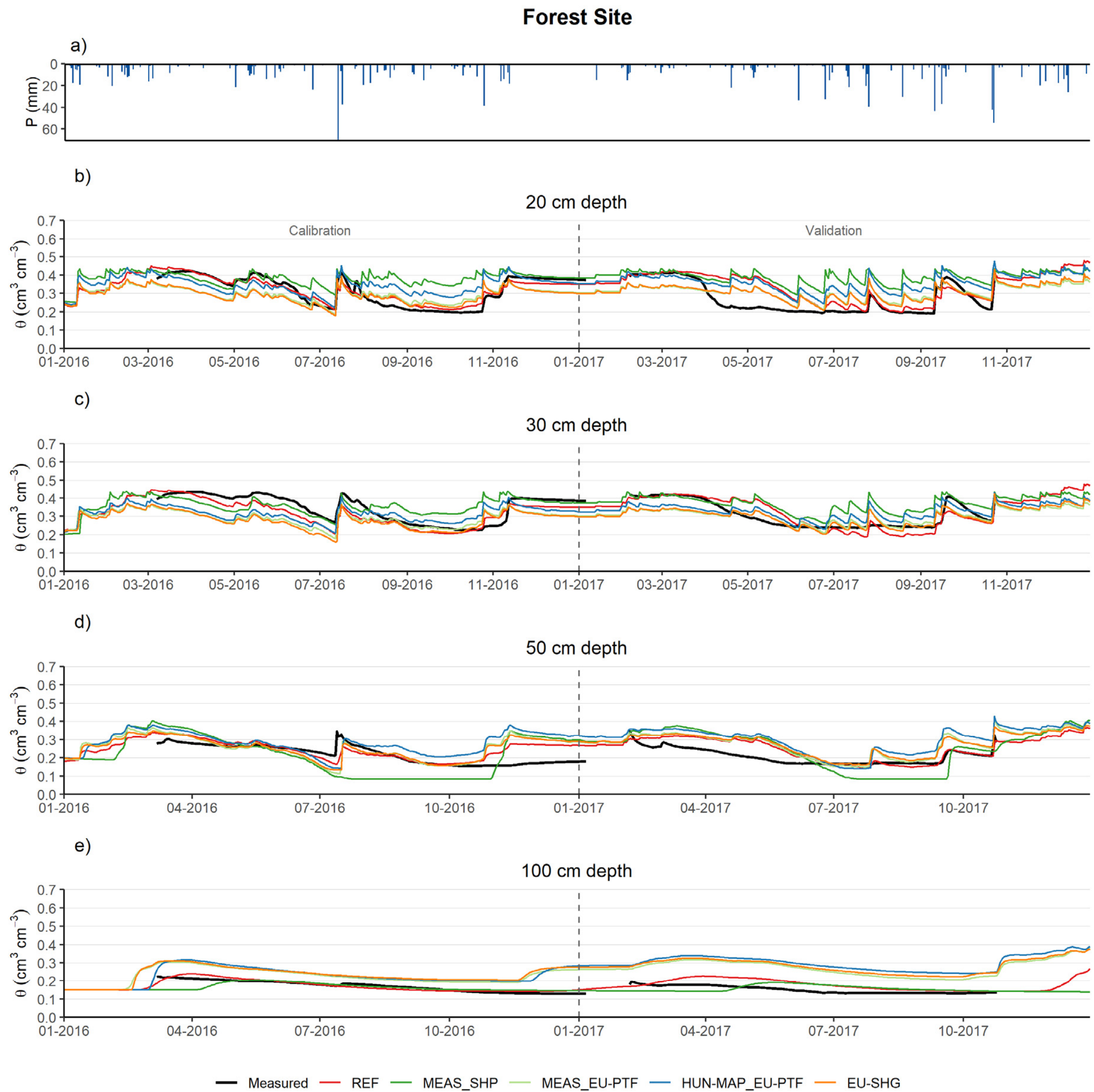


Fig. A11. Precipitation (a), measured and simulated soil moisture time series at the Forest Site for depths 20 cm (b), 30 cm (c), 50 cm (d) and 100 cm (e). Blank measured data indicate periods of low soil temperature, where measurements are not reliable.

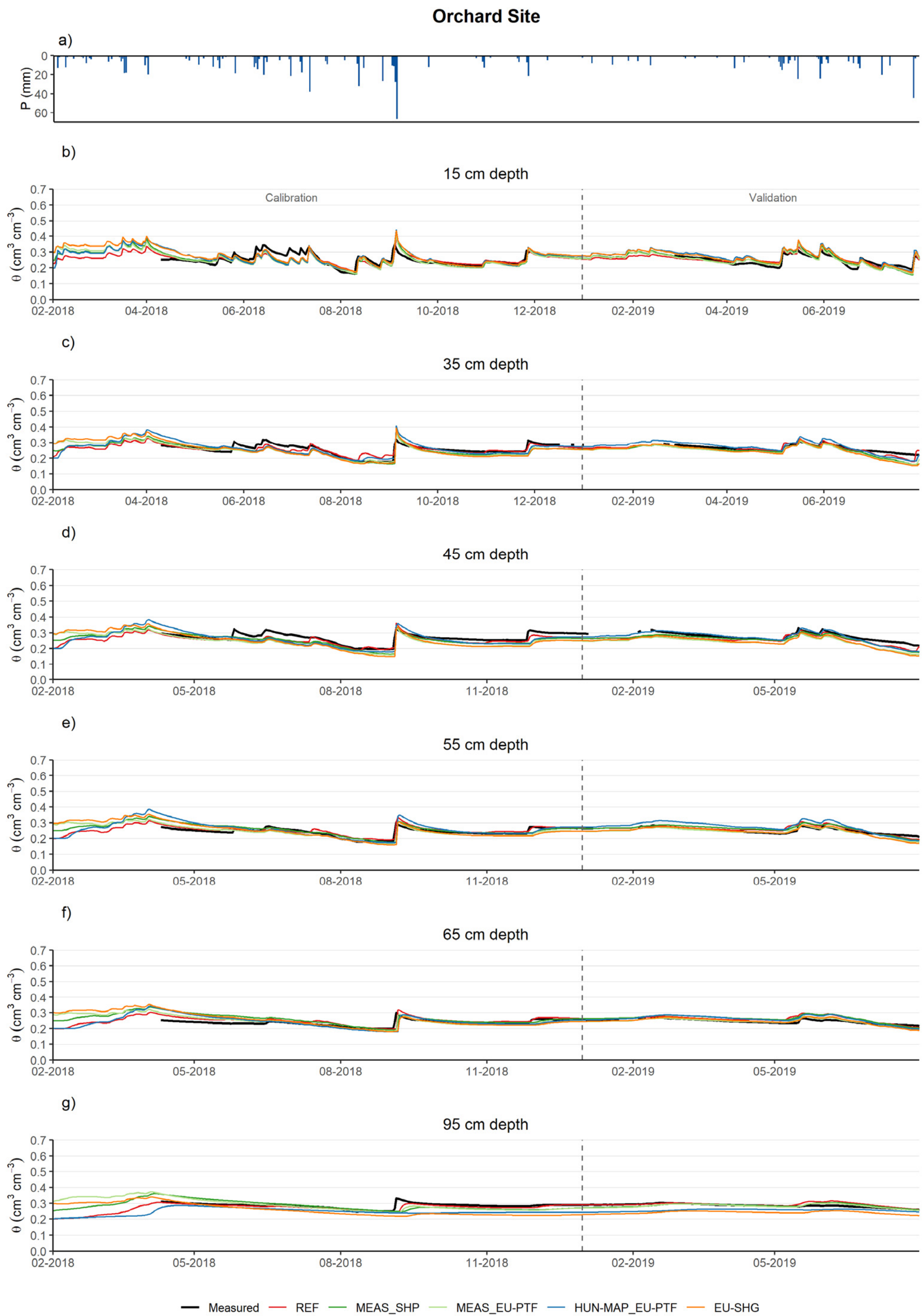


Fig. A12. Precipitation (a), measured and simulated soil moisture time series at the Orchard Site for depths 15 cm (b), 35 cm (c), 45 cm (d) 55 cm (e), 65 cm (f) and 95 cm (g). Blank measured data indicate periods of low soil temperature, where measurements are not reliable.

Model efficiency measures

$$R^2 = \left(\frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2 \sum_{i=1}^{n}(y_i - \bar{y})^2}}\right)$$

$$ME = \frac{\sum_{i=1}^{n}|x_i - y_i|}{n}$$

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

$$NSME = 1 - \frac{\sum_{i=1}^{n}(y_i - x_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y}_i)^2}$$

where R^2coefficient of determination
ME mean absolute error
RMSE root mean square error
NSME Nash-Sutcliffe model efficiency
x_i i-th value of simulated time series
y_i i-th value of measured time series
$\bar{x}, \bar{y}$ Average value of simulated/measured test time

Technical remarks

The process of Hydurs-1D model calibration was aided with the self-developed framework software "Batched Hydrologic Runs" (BHR.exe, (Decsi et al., 2020)). The BHR.exe serves as an extension for Hydrus-1D and carries out automated model set ups, model runs and statistical evaluation of results. It can be used for various calibration tasks (fitting of soil moisture at multiple depths, surface pressure head or bottom flux) and batched model runs with varying top-bottom boundary condition time series. Considering calibration, the main advantage of the BHR algorithm compared to the Hydrus-1D built in inverse solution is that not only soil hydraulic parameters, but practically all model input data can be optimized (involving e.g. vegetation data or soil layer positions). The BHR.exe carries out local/global optimizations by using the open source nlopt library (Johnson, 2014).