Final scientific report of research project KH-124765 entitled

"Development of new methodology for 3D soil hydraulic property mapping and testing its application on the catchment of Lake Balaton"

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Project period:	01/09/2017 – 31/08/2019
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Summary

We derived new soil hydraulic pedotransfer functions (PTFs) to compute the saturated water content (0 cm matric potential), field capacity (-330 cm matric potential), wilting point (-15 000 cm matric potential) with a performance close to other internationally accepted methods. The PTFs are random-forest-based and use basic soil properties and other environmental information as predictors. The PTFs were derived on the full Hungarian Detailed Soil Hydrophysical Database (MARTHA); therefore those are applicable to predict the soil hydraulic properties in the whole Pannonian region. We applied the PTFs to compute soil hydraulic properties for the catchment of Lake Balaton. Further to it we mapped the soil hydraulic properties with random-forest-based geostatistical methods as well and analysed the performance of the indirect (using PTFs) and direct (geostatistical) mapping methods. The benefit of maps prepared with random forest and kriging is that locally extreme values can be characterized better. In the case of pedotransfer-function-based mapping, it is advantageous that the calculation of uncertainty is much less computationally intensive than it is with geostatistical methods. The newly derived 3D soil hydraulic dataset is significantly more accurate than the previously available maps.

The new 3D soil hydraulic maps were used as input soil parameters and to define the Hydrologic Response Units for hydrological modelling of the Zala catchment. The rainfall-runoff processes of the catchment could be simulated in an adequate quality with the computed soil hydraulic properties.

The performance of the profile scale hydraulic simulations using computed soil hydraulic properties depended on the studied site. This was due to the sensitivity of the model to the soil hydraulic conductivity. The accuracy of the water retention curve described with the predicted van Genuchten parameters was appropriate. The saturated hydraulic conductivity, on the other hand, has to be measured and/or calibrated to properly simulate the temporal variation of soil moisture content and the components of the water budget.

The new PTFs and soil hydraulic maps are freely available from the website of the project (https://www.mta-taki.hu/en/kh124765).

Main results

1.1. Data collection of available static and time series information for the catchment scale modelling and start measurement of soil and vegetation parameters, soil moisture time series for the profile scale soil hydraulic simulations.

Catchment scale modelling

The catchment scale modelling was performed with the Soil and Water Assessment Tool (SWAT) (Neitsch et al., 2009). The model has been applied to the Zala catchment, which is the major tributary of Lake Balaton (Hungary) and has a long history of river monitoring, with reliable data sources. The area of the whole catchment is around 1500 km^2, with the outflow point at Zalaapáti. The average slope of the basin is 1.5 m/km, with large flat sections in the river valleys and floodplains and steeper hilly regions along the western part and the southern-central regions. The soils of the catchment comprise of three dominant soil texture class, silt loam at the west part, loam at the central-southern part, and sandy loam at the north-eastern part. The land use of the region is dominated by agriculture, but the western and some of the hillier southern parts have forest cover, mainly deciduous but mixed and evergreen forests are also present. For building the model the following datasets were collected: hydrometeorological time series, information on topography, land use, basic soil properties and soil hydraulic parameters.

Profile scale modelling

We used the Hydrus-1D software to carry out soil profile scale hydraulic simulations. The profiles were selected at Szalafő, Fiad, Keszthely and Vése (Figure 1). At Szalafő and Fiad sites soil moisture time series was provided by the Forest Research Institute of the National Agricultural Research and Innovation Centre. At Fiad site meteorological data was available from two nearby meteorological stations. We performed the soil profile description and laboratory analysis at all sites. Table 1 shows the measured soil hydraulic properties of the profiles. At Keszthely and Vése we installed the TDR/MUX/mpts meter (Easy Test) soil moisture probes and started the measurements in April 2018. At Vése water table sensor and meteorological station was installed as well.

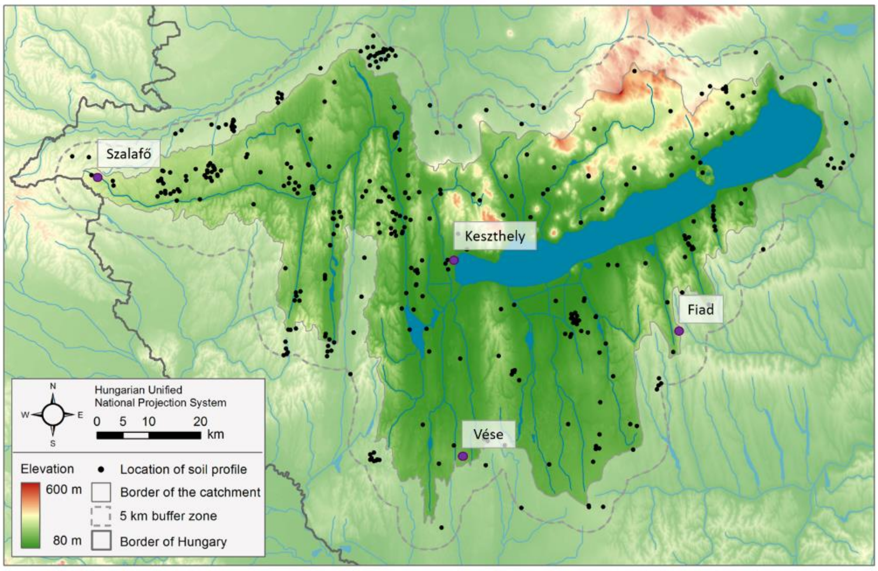

Figure 1. Location of soil moisture monitoring sites (Szalafő, Keszthely, Vése, Fiad) and soil profiles used for the geostatistical soil hydraulic mapping on the Balaton catchment study area.

Table 1. Soil hydraulic properties of the studied soil profiles.

Name of the site	Depth of sample (cm)	Soil water retention (cm^3 cm^{-3})										Saturated hydraulic conductivity (cm day^{-1})
		θ_0	$\theta_{2.5}$	θ_{10}	θ_{33}	θ_{100}	θ_{200}	θ_{330}	θ_{2500}	θ_{15000}	$\theta_{1500000}$	
Fiad	0-5	0.5469	0.5358	0.4996	0.4796	0.4672	0.4492	0.4400	0.1795	0.0999	0.0255	4.71
	17-22	0.4425	0.4373	0.4215	0.4104	0.3981	0.3805	0.3660	0.2201	0.1336	0.0325	4.75
	40-45	0.4517	0.4423	0.4214	0.4032	0.3795	0.3589	0.3424	0.2327	0.1490	0.0362	0.35
	75-80	0.5186	0.5089	0.4843	0.4515	0.3788	0.3236	0.2812	0.1614	0.0896	0.0181	10.00
Keszthely	5-10	0.4561	0.4466	0.4174	0.3885	0.3387	0.3007	0.2765	0.1428	0.0899	0.0164	15.65
	22-27	0.4063	0.4013	0.3756	0.3582	0.3212	0.2913	0.2734	0.1515	0.0979	0.0151	6.97
	42-47	0.3994	0.3948	0.3733	0.3599	0.3262	0.2960	0.2785	0.1594	0.1016	0.0162	10.43
	83-88	0.4736	0.4661	0.4394	0.4120	0.3613	0.3214	0.2961	0.1757	0.0884	0.0131	12.82
Szalafő	5-10	0.5670	0.5568	0.5292	0.5126	0.4897	0.4686	0.4525	0.2293	0.1388	0.0296	17.06
	25-30	0.4949	0.4828	0.4630	0.4488	0.4242	0.4047	0.3903	0.2258	0.1280	0.0259	77.04
	50-55	0.4671	0.4593	0.4351	0.4254	0.4067	0.3902	0.3759	0.2641	0.1705	0.0308	0.85
	65-70	0.4636	0.4530	0.4311	0.4225	0.4146	0.4041	0.3964	0.3004	0.1999	0.0488	0.38
Vése	5-15	0.4998	0.4866	0.4644	0.4566	0.4433	0.4167	0.3950	0.1390	0.0751	0.0201	44.33
	15-40	0.4294	0.4270	0.4051	0.3988	0.3801	0.3435	0.3178	0.1329	0.0735	0.0181	29.59
	40-60	0.3948	0.3924	0.3725	0.3635	0.3380	0.3130	0.2982	0.1330	0.0785	0.0168	3.79

1.2. Extension of the Hungarian Detailed Soil Hydrophysical Database (MARTHA).

The MARTHA database (Makó et al., 2010) was extended with soil chemical, physical and hydrological data of 145 soil horizons (Szabó et al., 2019a). 172 soil environmental variables were added to the dataset: topographical (70), meteorological (86), geological information (3), land cover (26) and remotely sensed vegetation (21) properties (Table 2). For wider applicability of the predictions derived on the dataset we worked on the harmonization of the particle size distribution data measured with different methods (Makó et al., 2017, 2019). The basic, chemical, physical and hydrologic properties of further 1143 soil profiles were collected from the database of the Forest Research Institute, National Agricultural Research and Innovation Centre.

Table 2. Environmental covariates added to the Hungarian Detailed Soil Hydrophysical Database (MARTHA).

Name	Resolution	Description
Parent material	1:100000	(Gyalog and Síkhegyi, 2005), map was converted to raster layer
Topography		
digital elevation model	25 m	(Bashfield and Keim, 2011) elevation, slope angle, aspect, northing and easting aspects, planar curvatures, profile curvatures, combined curvatures, topographic position indices, topographic position indices, terrain ruggedness indices, roughness, dissection, surface to area ratio, multi-resolution valley bottom flatness, multi-resolution ridge top flatness, negative openness, positive openness, convergence indices, LS factor, vector ruggedness measure, surface convexity, flow accumulation area, flow length, topographic wetness indices by single and multi-flow algorithms, vertical distance to existing water bodies, vertical distance to existing water bodies, horizontal distance to existing water bodies, smoothed version of elevation, smoothed version of profile curvature, smoothed version of slope, smoothed version of total curvature, standard deviations of elevation, standard deviations of profile curvature, standard deviations of slope, standard deviations of total curvature
Climate		
WorldClim	30”	(Fick and Hijmans, 2017) mean monthly temperature, precipitation, solar radiation, water vapour pressure, mean monthly minimum and maximum temperature
Hungarian data	100 m	(Szentimrey and Bihari, 2007) The spatial layers were compiled using the MISH method elaborated for the spatial interpolation of surface meteorological elements based on a 30 year observation by the Hungarian Meteorological Service with 0.5’ resolution. mean annual precipitation and temperature
State of vegetation		
MODIS	250 m	(Vermote, 2015) normalized difference vegetation index, near infrared, red
Land cover		
Copernicus Pan-European High Resolution Layers	20 m	(CEC EEA, 2012) tree cover density, forest type, impermeable cover of soil, wetland, grassland
CORINE Land Cover	25 ha	(CEC EEA, 2012) natural grassland, land principally occupied by agriculture

M1: The extended MARTHA ver3.0 database has been completed:

- the metadata is available from: https://www.mta-taki.hu/en/kh124765.

1.3. Deriving hydraulic pedotransfer functions

We derived hydraulic HUN-PTFs on the MARTHA ver3.0 database with random forest and generalized boosted regression model (Szabó et al., 2019a). Information on soil depth, soil properties and other environmental covariates - which are available for the Balaton catchment – were used as independent variables. Saturated water content (0 cm matric potential), field capacity (-330 cm matric potential), wilting point (-15 000 cm matric potential). The performance of the predictions is close to the performance of other internationally accepted PTFs (e.g. Botula et al. (2013), Román Dobarco et al. (2019), Zhang and Schaap (2017)) (Table 3).

Table 3. Performance of hydraulic PTFs on training and test datasets. THS: saturated water content, FC: field capacity, WP: wilting point, RF: random forest method, GBM: generalized boosted regression method, TEST_CHEM set: test dataset in which chemical soil properties are available for the predictions, TEST set: test dataset, in which chemical soil properties are not necessarily available for the predictions, RMSE: root mean square error, R^2: determination coefficient.

Predicted soil hydraulic property		Selected method*	Train set**			TEST set			TEST_CHEM set		
			R^2	RMSE ($cm^3\ cm^{-3}$)	N	R^2	RMSE ($cm^3\ cm^{-3}$)	N	R^2	RMSE ($cm^3\ cm^{-3}$)	N
THS	topsoil	GBM	0.453	0.052	5709	-	-	-	0.484	0.042	2448
		RF	0.488	0.041	5709	-	-	-	0.487	0.042	2448
	subsoil	GBM	0.429	0.045	8428	0.418	0.045	3611	0.400	0.046	2448
		RF	0.480	0.043	8428	0.429	0.045	3611	0.408	0.045	2448
FC	topsoil	GBM	0.714	0.043	5635	-	-	-	0.770	0.039	2416
		RF	0.736	0.041	5635	-	-	-	0.766	0.039	2416
	subsoil	GBM	0.738	0.044	8352	0.739	0.042	3579	0.751	0.040	2416
		RF	0.756	0.042	8352	0.746	0.042	3579	0.759	0.040	2416
WP	topsoil	GBM	0.722	0.038	5736	-	-	-	0.739	0.037	2459
		RF	0.736	0.037	5736	-	-	-	0.762	0.035	2459
	subsoil	GBM	0.717	0.041	8425	0.716	0.039	3611	0.711	0.038	2459
		RF	0.747	0.039	8425	0.737	0.038	3611	0.744	0.036	2459

* Input parameters included in all analysis for topsoils: soil type according to Hungarian classification system, sand (50–2000 μm), silt (2–50 μm) and clay content (<2 μm) ($100\ g\ g^{-1}$), mean depth (cm) and information on topography, vegetation, meteorology and parent material listed in Table 1. For subsoils organic matter content ($100\ g\ g^{-1}$); pH in water and calcium carbonate content ($100\ g\ g^{-1}$) were included as well.
** Prediction error calculated on training is based on out of bag error in case of RF and 5-fold cross-validation in case of GBM method.

The MARTHA dataset does not include measured data on the unsaturated hydraulic conductivity, therefore the estimation of the Mualem-van Genuchten model parameters of the moisture retention and hydraulic conductivity curve were predicted with EU-PTFs (euptfv1) (Tóth et al., 2015) for the catchment of Lake Balaton.

For future use we derived new parametric PTFs with random forest method (Szabó et al., 2019b) on the European Hydropedological Data Inventory (EU-HYDI) (Weynants et al., 2013). The updated EU-PTFs – euptfv2 – perform significantly better than euptfv1 and are applicable for 32 predictor variables combinations. Uncertainties of the predicted soil hydraulic properties and model parameters can be computed. These uncertainties are, without further discrimination, related to the considered input data, predictors and the applied algorithm. The algorithms are available from a user friendly web interface (Szabó et al., 2019c).

M2: The derived PTFs are freely available from the website of the from the Institute for Soil Sciences and Agricultural Chemistry Centre for Agricultural Research:

- region specific point HUN-PTFs: https://www.mta-taki.hu/en/kh124765/hun_ptfs
- parametric PTFs: https://ptfinterface.rissac.hu

1.4. 3D mapping of soil hydraulic properties for the catchment of Lake Balaton.

We derived the 3D soil hydraulic maps at 100 m resolution both with the HUN-PTFs and geostatistical (RFK) methods (Szabó et al., 2019a). With the HUN-PTFs method we mapped the uncertainty of the computed soil hydraulic properties as well. Figures 2-4 show the new and previously available (EU-SoilHydroGrids) soil hydraulic maps of the catchment.

There were no significant differences between the direct and indirect methods in six out of nine maps having root-mean-square-error values between 0.052 and 0.074 cm^3 cm^{-3}. HUN-PTFs performed significantly better for the prediction of saturated water content at 30-60 and 60-90 cm depth, in the case of wilting point the RFK outperformed the PTFs at 60–90 cm depth. Although the absolute difference between the RFK and HUN-PTFs maps is less than 0.025 cm^3 cm^{-3} for at least 75 % of the area. Spatial patterns of topography are less dominant on the soil hydraulic maps prepared by the RFK method due to kriging the residuals, which is an advantage. If only the most probable soil hydraulic value is needed for the Balaton catchment area, it is suggested to use the soil hydraulic maps prepared by the RFK. If information on uncertainty is needed as well, maps derived by the HUN-PTFs are recommended.

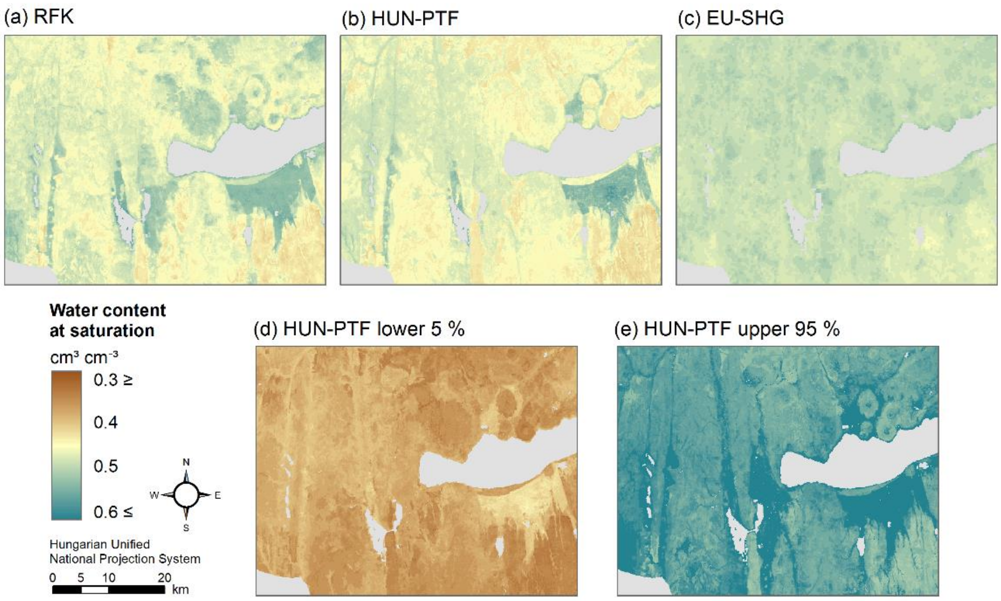

Figure 2. Map of water content at saturation in 0-30 cm soil depth derived by random forest and kriging mapping approach (RFK) (a), Hungarian pedotransfer functions (HUN-PTF) (b) and cut from the EU-SoilHydroGrids 250m dataset (EU-SHG) (c), possible lower 5 % (d) and upper 95 % (e) based on HUN-PTF for a section of the Balaton catchment.

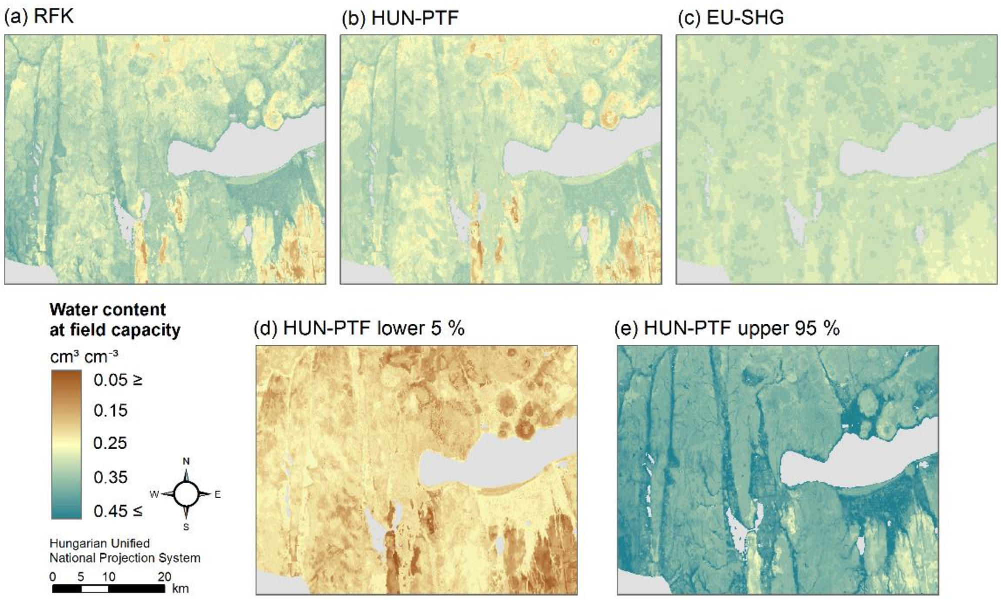

Figure 3. Map of water content at field capacity in 0-30 cm soil depth derived by random forest and kriging mapping approach (RFK) (a), Hungarian pedotransfer functions (HUN-PTF) (b) and cut from the EU-SoilHydroGrids 250m dataset (EU-SHG) (c), possible lower 5 % (d) and upper 95 % (e) based on HUN-PTF for a section of the Balaton catchment.

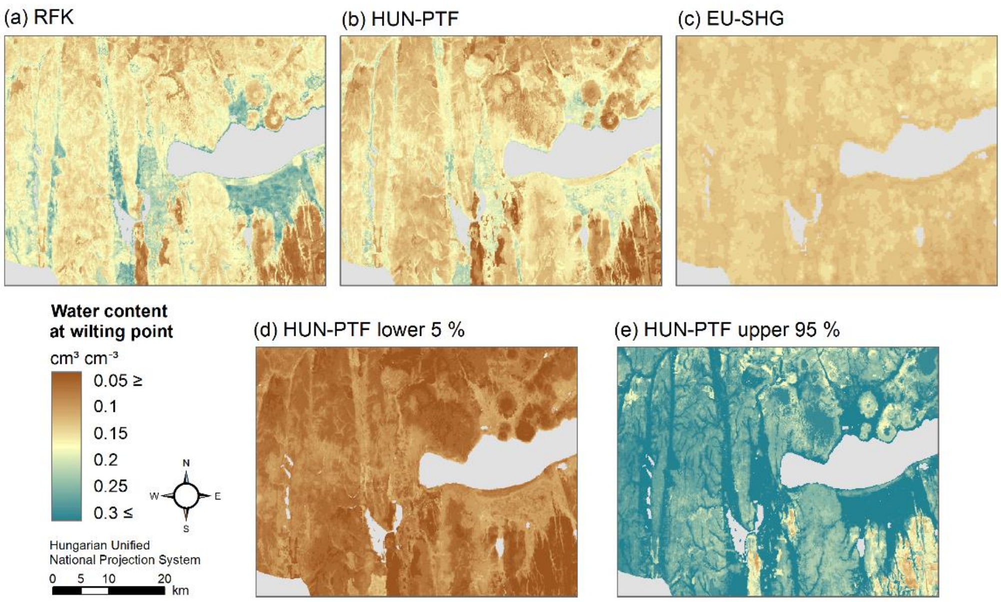

Figure 4. Map of water content at wilting point in 0-30 cm soil depth derived by random forest and kriging mapping approach (RFK) (a), Hungarian pedotransfer functions (HUN-PTF) (b) and cut from the EU-SoilHydroGrids 250m dataset (EU-SHG) (c), possible lower 5 % (d) and upper 95 % (e) based on HUN-PTF for a section of the Balaton catchment.

2.1. Providing soil hydraulic data from national and continental sources for the hydrological models.

Catchment scale modelling

The SWAT simulation was done with two model variants, which differed only in the source dataset of soil input parameters (Table 4). Model 1 used solely European open access soil datasets: the SoilGrids and EU-SoilHydroGrids. In Model 2 regional and national soil dataset were included, namely the new 3D soil hydraulic maps (Szabó et al., 2019a) derived in 1.4 task of the project and the DOSoReMI.hu dataset (Pásztor et al., 2018). The map of saturated hydraulic conductivity and bulk density was derived with the HUN-PTF method.

Table 4. Soil data sources used for the two SWAT model variants.

Soil data	Model 1 – European dataset (250 m)	Model 2 – Regional/National dataset (100m)
Available water content (AWC)	EU-SoilHydrogrids (Tóth et al., 2017a)	3D soil hydraulic datset for the catchment of Lake Balaton (Szabó et al., 2019a)
Saturated hydraulic conductivity (Ksat)	EU-SoilHydrogrids	derived with HUN-PTF method
Clay,silt,sand content	SoilGrids (Hengl et al., 2017)	DOSoReMI (Pásztor et al., 2018)
Bulk density	SoilGrids	derived with HUN-PTF method
Maximum rooting depth	SoilGrids	DOSoReMI
Soil taxonomical information	SoilGrids	DOSoReMI
Organic carbon content	SoilGrids	DOSoReMI

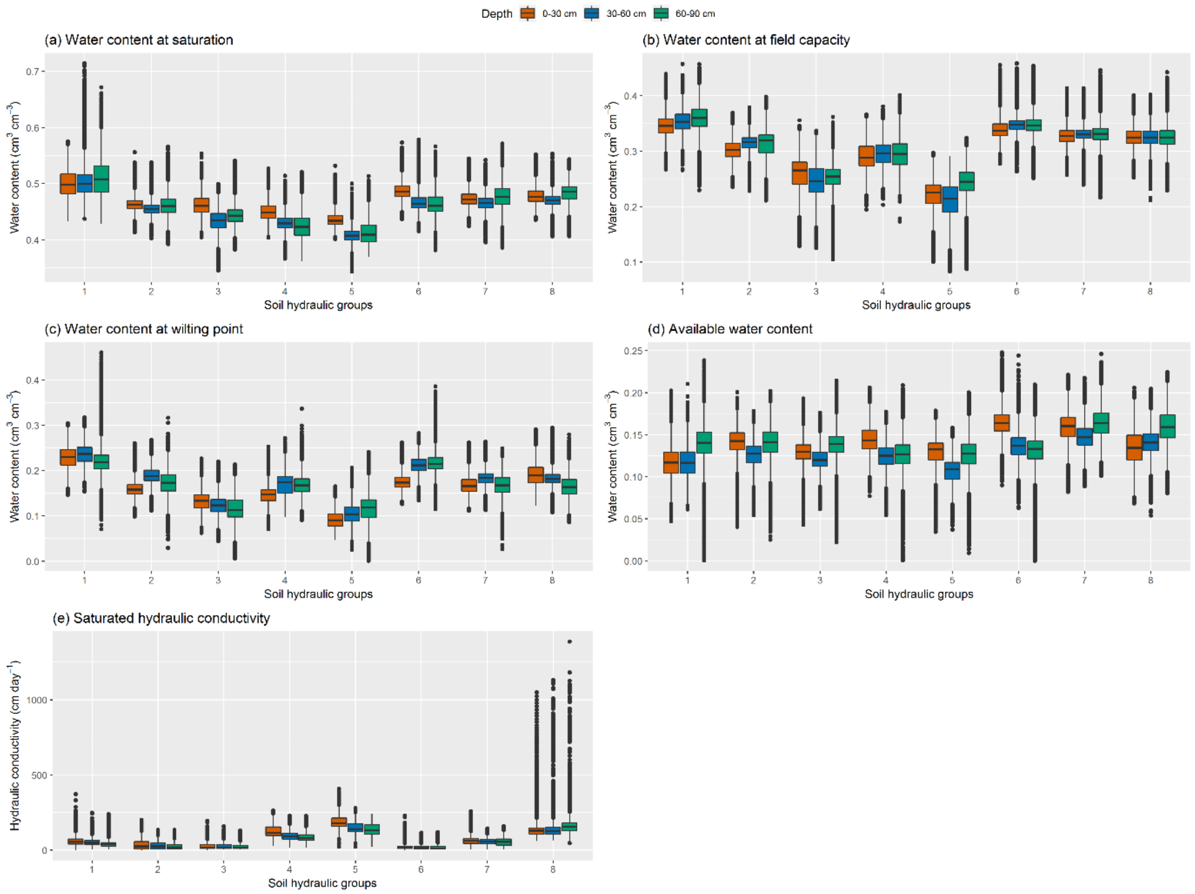

Figure 5. Characteristics of soil hydraulic groups computed with k-means clustering of the soil hydraulic maps derived by random forest and kriging approach (RFK).

For the SWAT model we analysed how the newly derived soil hydraulic maps could be used to define the Hydrological Response Units. We derived Soil Hydraulic Groups with k-means clustering (Laborczi et al., 2019; Szabó et al., 2020) of the newly derived 3D soil hydraulic maps of the Balaton catchment (Figure 5) and EU-SoilHydroGrids dataset.

Profile scale modelling
We computed the Mualem-van Genuchten parameters with EU-PTFs (euptfv1) (Tóth et al., 2015) for the catchment of Lake Balaton for the 0-30, 30-60 and 60-90 cm soil depths at a 100 m horizontal resolution and extracted the parameters from those maps for the locations of the analysed soil profiles. Figure 6 shows the density plots of the mapped parameter values. The θ_r, θ_s, α and n parameters were computed with the class PTF (PTF19), which considers USDA texture classes and topsoil/subsoil distinction, the saturated hydraulic conductivity was computed with regression-tree-based PTF (PTF16) (Tóth et al., 2015), therefore the density plots of these soil hydraulic parameters have multiple peaks within the same soil depth.

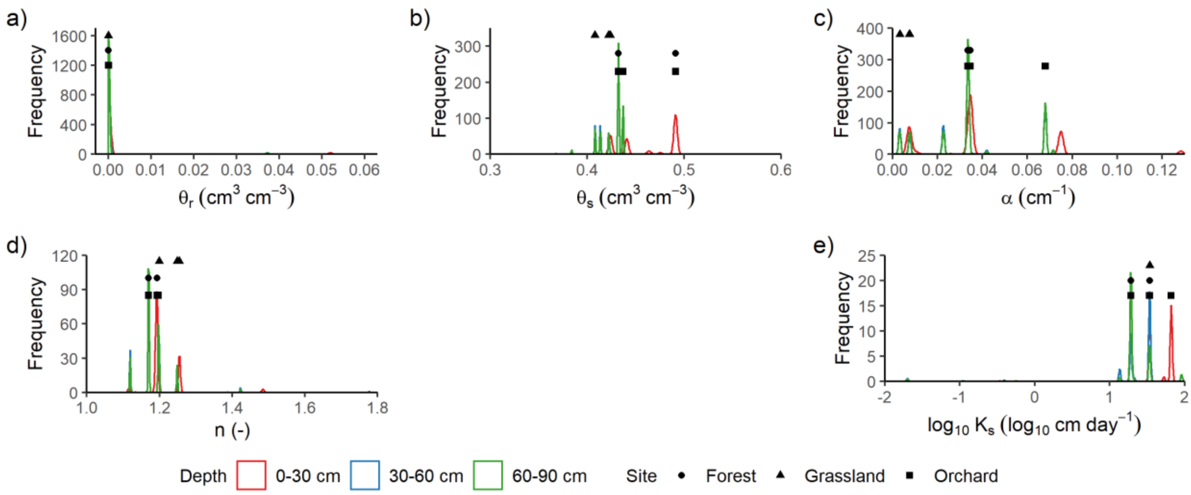

Figure 6. Density plots of a)-d) mapped van Genuchten model parameters to describe the soil moisture retention curve and e) saturated hydraulic conductivity for the area of Balaton catchment by soil depths and the parameters of the three sites. Maps were derived by applying EU-PTFs on the soil map information of the DOSoReMI.hu (HUN-MAP_EU-PTF). θ_r: residual water content; θ_s: saturated water content; α and n: fitting parameters; K_s: saturated hydraulic conductivity.

2.2. Comparing performance of soil hydraulic maps

New 100m resolution soil hydraulic maps significantly outperformed the EU-SoilHydroGrids (Table 5), which was expected because (i) reference soil data originate from the mapped area and also (ii) spatially denser and (iii) locally trained models are used. In addition, several environmental covariates were considered for the predictions and relationship between easily available soil properties, and soil hydraulic parameters were derived from local data.

Table 5. Performance of soil hydraulic maps derived by random forest and kriging method (RFK), Hungarian pedotransfer functions (HUN-PTF) and from EU-SoilHydroGrids 250m dataset (EU-SHG) on the Balaton catchment. RMSE: root mean square error, SS_{mse}: mean square error skill score.

Predicted soil hydraulic property	Depth	Method	N	RMSE ($cm^3\ cm^{-3}$)	SS_{mse}	Sign. difference*
THS	0-30 cm	RFK	324	0.056	0.382	b
		HUN-PTF	350	0.067	0.118	b
		EU-SHG	348	0.070	0.041	a
	30-60 cm	RFK	321	0.060	0.119	a
		HUN-PTF	345	0.058	0.150	b
		EU-SHG	343	0.063	-0.004	a
	60-90 cm	RFK	315	0.063	0.112	b
		HUN-PTF	337	0.060	0.171	c
		EU-SHG	335	0.071	-0.149	a
FC	0-30 cm	RFK	324	0.053	0.547	b
		HUN-PTF	350	0.067	0.265	b
		EU-SHG	348	0.076	0.070	a
	30-60 cm	RFK	321	0.057	0.515	b
		HUN-PTF	345	0.069	0.278	b
		EU-SHG	343	0.084	-0.069	a
	60-90 cm	RFK	315	0.062	0.485	b
		HUN-PTF	337	0.074	0.232	b
		EU-SHG	335	0.095	-0.243	a
WP	0-30 cm	RFK	324	0.052	0.453	b
		HUN-PTF	349	0.062	0.244	ab
		EU-SHG	347	0.071	-0.038	a
	30-60 cm	RFK	321	0.052	0.467	b
		HUN-PTF	344	0.065	0.152	b
		EU-SHG	342	0.074	-0.112	a
	60-90 cm	RFK	315	0.057	0.443	c
		HUN-PTF	335	0.067	0.208	b
		EU-SHG	333	0.076	-0.026	a

*Different letters indicate significant differences at 0.05 level between the accuracy of the methods based on squared error, e.g. performance indicated with letter c is significantly better than the one noted with letter b and a.

In Szabó et al. (2019a) we highlight the most important differences between pedotransfer-function-based (HUN-PTF) and geostatistical (RFK) soil hydraulic mapping based on the Balaton catchment.

The RMSE values of the MRC computed based on the mapped van Genuchten parameters are around 0.07 $cm^3\ cm^{-3}$ for HUN-MAP_EU-PTF and 0.07-0.09 $cm^3\ cm^{-3}$ for EU-SHG (Table 6) analysed on the samples with measured theta-head pairs of Balaton catchment. 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 0.054-0.067 $cm^3\ cm^{-3}$ for PTF19 and 0.046 $cm^3\ cm^{-3}$ for PTF22. In case of both maps PTF16 of EU-PTFs was used to compute the saturated hydraulic conductivity. 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 smaller, 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 on only 35-37 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.

Table 6. Performance of soil hydraulic maps computed for the Balaton catchment based on the measured profile data of the Hungarian Detailed Soil Hydrophysical Dataset. K_S: 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 (cm)**	**K_S ($\log_{10}$ (cm day^{-1}))**			**MRC (cm^3 cm^{-3})**		
		ME	**RMSE**	**N**	**ME**	**RMSE**	**N**
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

2.3. Set up, calibration and validation of catchment and profile scale models.

Catchment scale modelling

The Zala catchment has been divided into 46 subbasins. HRUs are generated within the subbasins therefore subbasin number also determines the amount of HRUs in the model. A 5% threshold was used to reduce the amount of HRUs in the model, in this way soil class or land use type or slope class with less than 5% of the total area of a subbasin are neglected, and the area of them is redistributed between the other classes proportionally. As a result of different soil input datasets, the two model variants were structured with different numbers of HRUs (Table 7). For Model 2 we used the Soil Hydraulic Groups derived in task 2.1.

Table 7. Information used to derive the Hydrological Response Units (HRU) for the two SWAT model variants.

Data description	**Model 1 – European dataset (250 m)**	**Model 2 – Regional/National dataset (100m)**
Soil classes	WRB Reference Groups	Soil Hydological Groups
Land use	Corine land cover	
Slope classification	6 slope classes	
Total HRU number	4400 HRUs	6700 HRUs
HRU number after applying the 5% treshold values	1050 HRUs	1756 HRUs

There are several settings and options for the model, which affects the model results. Without giving full details, the essential settings are introduced: the evapotranspiration was calculated using the Penman-Monteith and the Hargreaves methods (Neitsch et al., 2009). For runoff calculation, the SCS curve number method was used (Neitsch et al., 2002). The variable storage flow routing option was used, and the model was run with daily time steps.

Model sensitivity analysis, calibration, and validation

The SWAT model has been calibrated with the SWAT-CUP SUFI2 software (Abbaspour, 2015), specifically designed to calibrate SWAT model applications. The calibration has been delivered in a protocol suggested by the program developers (Abbaspour et al., 2015). Global sensitivity analysis has been used parallel to the calibration of the model parameters. It gives a rank of model parameter sensitivity relative to each other. Therefore the number of the model parameters included in the analysis, as well as the selection of the parameters, does have an impact on the results of the ranking and the sensitivity itself. The parameters included in the sensitivity analysis have been shuffled, adding, and removing parameters according to the results of each iteration. Model parameters have been calibrated by land use class (CN values), soil texture class (soil hydraulic parameters) and soil layers (soil hydraulic parameters).

The Nash-Sutcliff model efficiency (NSME) has been used as objective function for the calibration. Daily flow data of the Zalaapáti river gauge have been used for calibration. Model calibration covered the 1994-2003 period. Warm-up of 3 years has been used to initialize the model and to reduce errors arising from inaccurate initial conditions. Validation has been done for the 2001-2010 period with 3 years warmup period as well.

Beside NSE, other indicators have been used to compare model results. Coefficient of determination and the P and R factors are used for this purpose. The P factor gives the percentage of the measured flow values within the 95% uncertainty interval for the calculated values (P = 1 gives the highest match). The R values represent the mean width of the uncertainty interval, divided by the standard deviation value; the closer the R value is to 0, the better the model performance. The V_f value is the volumetric fraction of the total calculated runoff and the total simulated runoff.

Results of uncertainty analysis for the two model variants

The results of the model applications show slight differences in model parameter sensitivity and model performance values (Jolánkai et al., 2019). In both model variants, the model performs satisfactorily but at a moderate level (Table 8.). Both in the calibration and validation period, there are very wet years followed by dry ones, therefore the model accuracy drops as high flows are generally underestimated at extreme conditions. Interestingly the validation of the model shows a better performance, which might be due to more stable hydrologic conditions over the years. Among the soil hydraulic properties saturated hydraulic conductivity and available soil water capacity were the key parameters required by the calibration in both model variants (Table 9.).

Table 8. Modell efficiency computed for the calibration and validation periods of the two model variants.

Modell efficiency	Model 1 – European dataset		Model 2 – Regional/National dataset	
	Calibration	**Validation**	**Calibration**	**Validation**
NSME	0.52	0.60	0.55	0.59
P	0.35	0.70	0.48	0.63
R	0.33	0.72	0.33	0.48
R^2	0.57	0.61	0.55	0.59
V_f	1.18	1.07	1.00	0.96

Table 9. Sensitivity of the SWAT parameters in descending order. Definitions of variables are found in the SWAT user manual (http://swatmodel.tamu.edu/documentation).

Model 1 – European dataset (250 m)	Model 2 – Regional/National dataset (100m)
• soil evaporation compensation factor	• saturated hydraulic conductivity of the soil ($l_{1\text{-}5}$)
• saturated hydraulic conductivity of the soil ($l_{1\text{-}5}$)	• available soil water capacity ($l_{1,2}$)
• available soil water capacity ($l_{2\text{-}6}$)	• SCS runoff curve number for moisture condition II – AGRR
• Manning’s n value for the main channels - AGRL	• groundwater ’revap’ coefficient
• SCS runoff curve number – AGRR	• Depth from soil surface to bottom of layer (l_4)
• delay time for aquifer recharge	• Manning’s n value for the main channels
• deep aquifer percolation fraction	• Manning's n value for overland flow

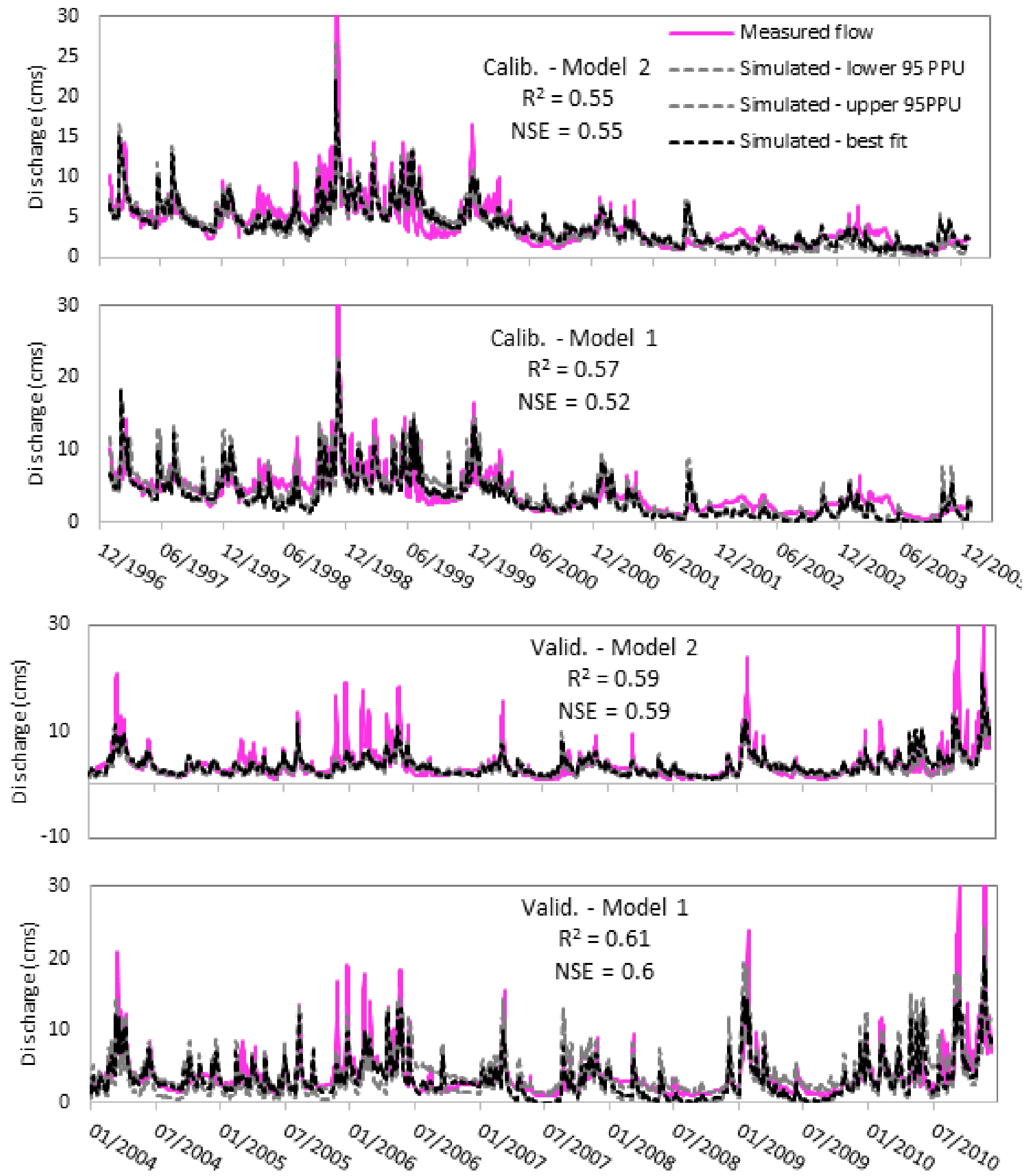

Figure 7. Calibration and validation results for the Zalaapáti gauge for the two model variants.

Spatial distribution of water balance

Another way to estimate differences between the two model variants is the spatial comparison of the water balance components, i.e., surface runoff (SURQ), lateral flow (LATQ), and groundwater flow (GWQ). The calibrated models with both model variants show spatial similarity in general (Figure). Both models generate very little surface runoff (2-3 % of the total runoff), which is the primary reason for moderate calibration results. Lower threshold for urban areas would increase surface runoff as in the current model many of the sealed surfaces are removed by the threshold. The surface runoff components are higher on this catchment, around 10-20% of the total runoff, as it was determined by digital baseflow separation earlier (Jolánkai and Koncsos, 2018). Only sealed surfaces generate higher runoff values according to the model. Hilly areas with steeper slopes are dominated by lateral flow (interflow or fast subsurface flow in other words) according to both models, with only minor differences in the spatial patterns. The distribution of groundwater flow shows strong similarities as well. In river valleys, flood plains, and areas with smaller slopes, the primary source of runoff is groundwater flow (GWQ – Figure 8).

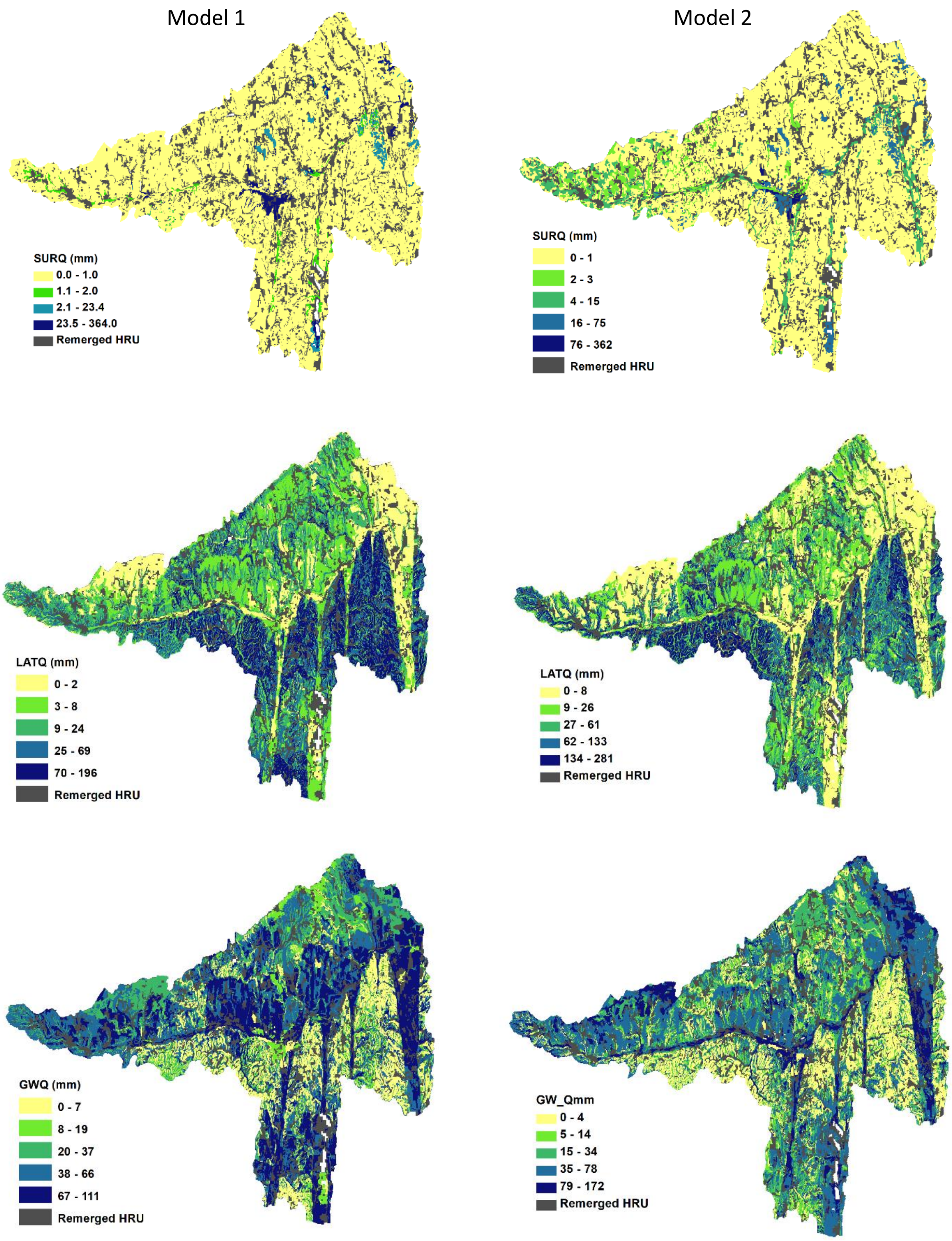

Figure 8. – Spatial distribution of runoff components as a result of two model variants (SURQ – surface runoff, LATQ – lateral flow or interflow, GWQ - groundwater flow).

Profile scale modelling

Five soil-vegetation-atmosphere models were set up with Hydrus-1D model for Szalafő, Fiad and Keszthely sites, differing only in the parametrization of input soil data (Kozma et al., 2019b). Beside the 1) reference model variant (REF), in which measured and calibrated values were used, we analysed the following soil hydraulic properties: 2) measured in the laboratory (MEAS_SHP), 3) predicted from the measured basic soil properties with the 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 (HUN-MAP_EU-PTF), 5) retrieved from the 250 m resolution EU-SoilHydroGrids dataset (Tóth et al., 2017a) (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 (Kozma et al., 2019a). Therefore, we considered this variant as the best achievable approximation of the soil-water fluxes computed by the Hydrus-1D simulation. The 2)-5) model variants were derived from the REF.

In Vése site there were some periods, when meteorological data were not registered due to unforeseen problems with the data logger; therefore we will simulate the temporal variation of the soil moisture content after having measured the next vegetation period as well. The specificity of the site is that the water table strongly influences the water budget of the profile. Soil moisture time series of similar sites are rarely monitored in Hungary, thus the monitoring and analysis of the Vése site will provide important results.

Calibration-validation, modell efficiency

Automated calibration was applied only for the (1) REF model variant. Standard measures of goodness-of-fit (R^2, Root Mean Square Error - RMSE, Mean Absolute Error – MAE, Nash-Sutcliffe Model Efficiency - NSME) were used to quantify the agreement between measured and simulated soil moisture time series.

The process of calibration was aided with the self-developed framework software "Batched Hydrologic Runs" (BHR.exe) (Kozma et al., 2014). 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). The BHR.exe carries out local/global optimizations by using the open source nlopt (Johnson, 2014) library.

Simulation of soil moisture

According to the guidelines of Harmel et al. (2018), the calibration-validation at the Forest and Orchard Site can be considered as acceptable, and it was outstanding for the Grassland Site. Figure 9. shows measured and simulated time series with the amount pf precipitation for the Grassland Site. The calibrated soil parameters (REF) led to the best model performance at all locations, NSME was 0.49, 0.54 and 0.75 for the Forest, Orchard and Grassland Site respectively (Table 10).

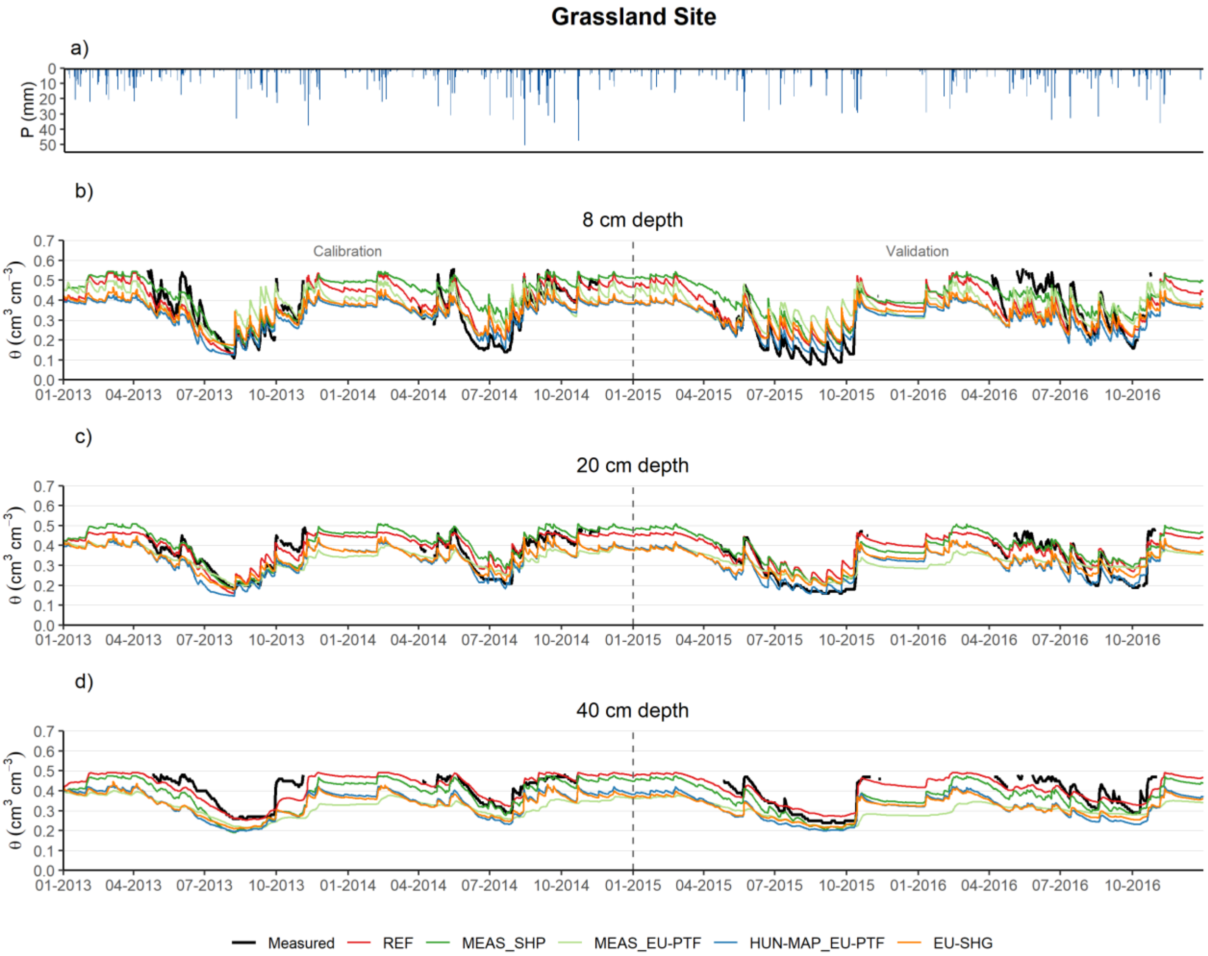

Figure 9. Amount of precipitation (a) and measured and simulated soil moisture content time series data (b-d) at Grassland Site for the 2013-2014 calibration (NSME = 0.75) and 2015-2016 validation (NSME = 0.70) periods.

Table 10. 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. Dimension: NSME [-], RMSE [$cm^3\ cm^{-3}$], ME [$cm^3\ cm^{-3}$], R^2 [-].

Name of the site		Goodness-of-fit by model variants					Number of measured soil moisture content per soil layer	Calibration period	Validation period
		REF	MEAS_SHP	MEAS_EU-PTF	HUN-MAP_EU-PTF	EU-SHG			
Forest Site	NSME	0.49	-0.94	-0.29	-0.35	0.13	568	01/01/2016-31/12/2016	01/01/2017-31/12/2017
	RMSE	0.04	0.09	0.07	0.07	0.06			
	MAE	0.03	0.06	0.07	0.08	0.07			
	R^2	0.77	0.50	0.70	0.69	0.59			
Orchard Site	NSME	0.54	0.15	0.07	-0.30	-0.69	391-478	01/02/2018-31/12/2018	01/01/2019-31/07/2019
	RMSE	0.02	0.02	0.02	0.03	0.03			
	MAE	0.01	0.02	0.02	0.02	0.03			
	R^2	0.86	0.74	0.79	0.68	0.70			
Grassland Site	NSME	0.74	0.23	0.46	0.39	0.66	760-817	01/01/2013-31/12/2014	01/01/2015-31/12/2016
	RMSE	0.04	0.08	0.06	0.07	0.05			
	MAE	0.04	0.06	0.08	0.08	0.07			
	R^2	0.89	0.83	0.84	0.88	0.89			

For all three sites the MEAS_SHP model variant had the lowest mean absolute error for most of the studied period (Figure 10). For the Forest and Orchard Site the MEAS_EU-PTF model variant provided

the second most accurate simulation. If only validation period is considered, MEAS_EU-PTF outperformed the MEAS_SHP. When soil parameters were derived from open access soil datasets, 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. Interestingly, at 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.
The soil moisture time series simulated with predicted soil hydraulic parameters are almost parallel for each site.

In the Forest Site the soil moisture content was underpredicted in wetter periods, and overpredicted in drier periods. Overprediction occurred more frequently especially at 20 and 30 cm depths. The correlation coefficients between the measured and simulated soil moisture content values were between 0.37 and 0.85. The lower values were obtained for 100 cm soil depth, MEAS_SHP performed the worst and EU-SHG the best.

In the Orchard Site the variability of soil moisture content was the smallest among the three sites, due to smallest amount of precipitation in the studied period. Underprediction of soil moisture time series occured in wet periods. Overprediction was not characteristic. The highest prediction error occurred in the wettest period (09-2018) of the simulation, in the deeper layer soil moisture content was underpredicted, in the top 35 cm it was overpredicted in that period in the case of all model variants. Correlation coefficients between the observed and simulated time series with predicted soil hydraulic properties were between 0.35 and 0.89. Lower values (0.35-0.62) were obtained at 95 cm soil depth.

In the Grassland Site in the case of all model variants overprediction occurs when the soil starts to dry out and in dry periods (Figure 11). Underprediction is characteristic, when the moisture content of the soil is close to saturation. At 8 cm depth, MEAS_SHP and MEAS_EU-PTF usually overpredicts the soil moisture content, in contrast HUN-MAP_EU-PTF and EU-SHG underpredicts the soil moisture content in most of the studied period. Except in the case of MEAS_SHP, at 20 cm depths mainly underprediction occurs with all model variants. At 40 cm depth all model variant underestimates the soil moisture time series.

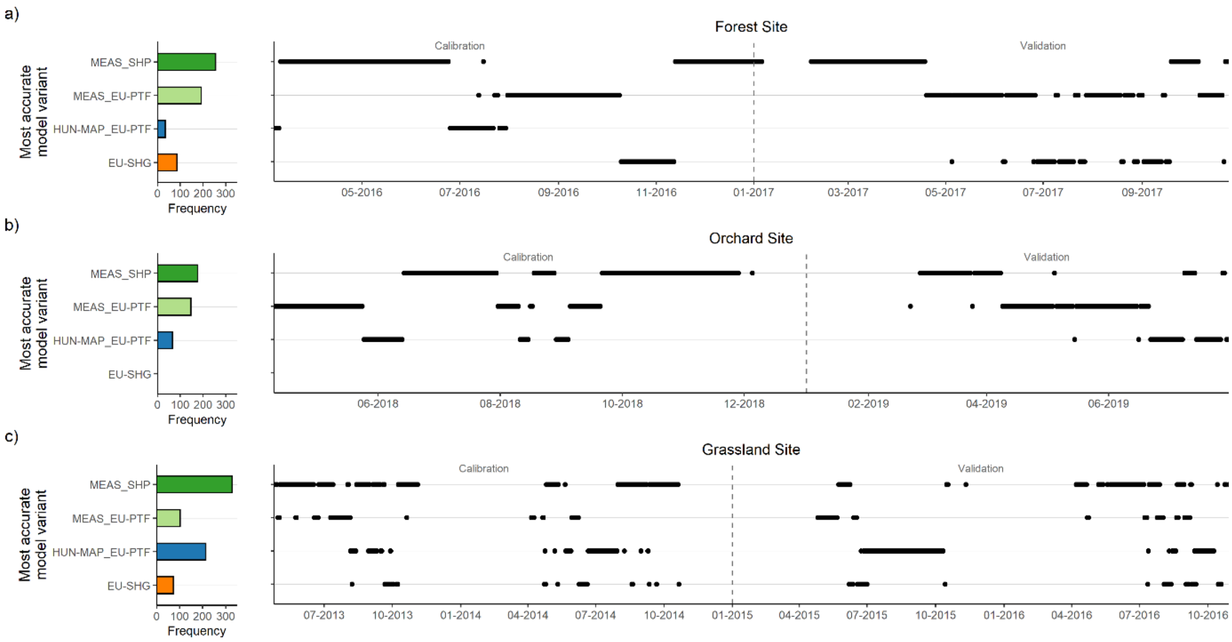

Figure 10. The most accurate model variants based on mean absolute error of the simulated soil moisture content, computed by day for the whole soil profile in the a) Forest, b) Orchard and c) Grassland sites.

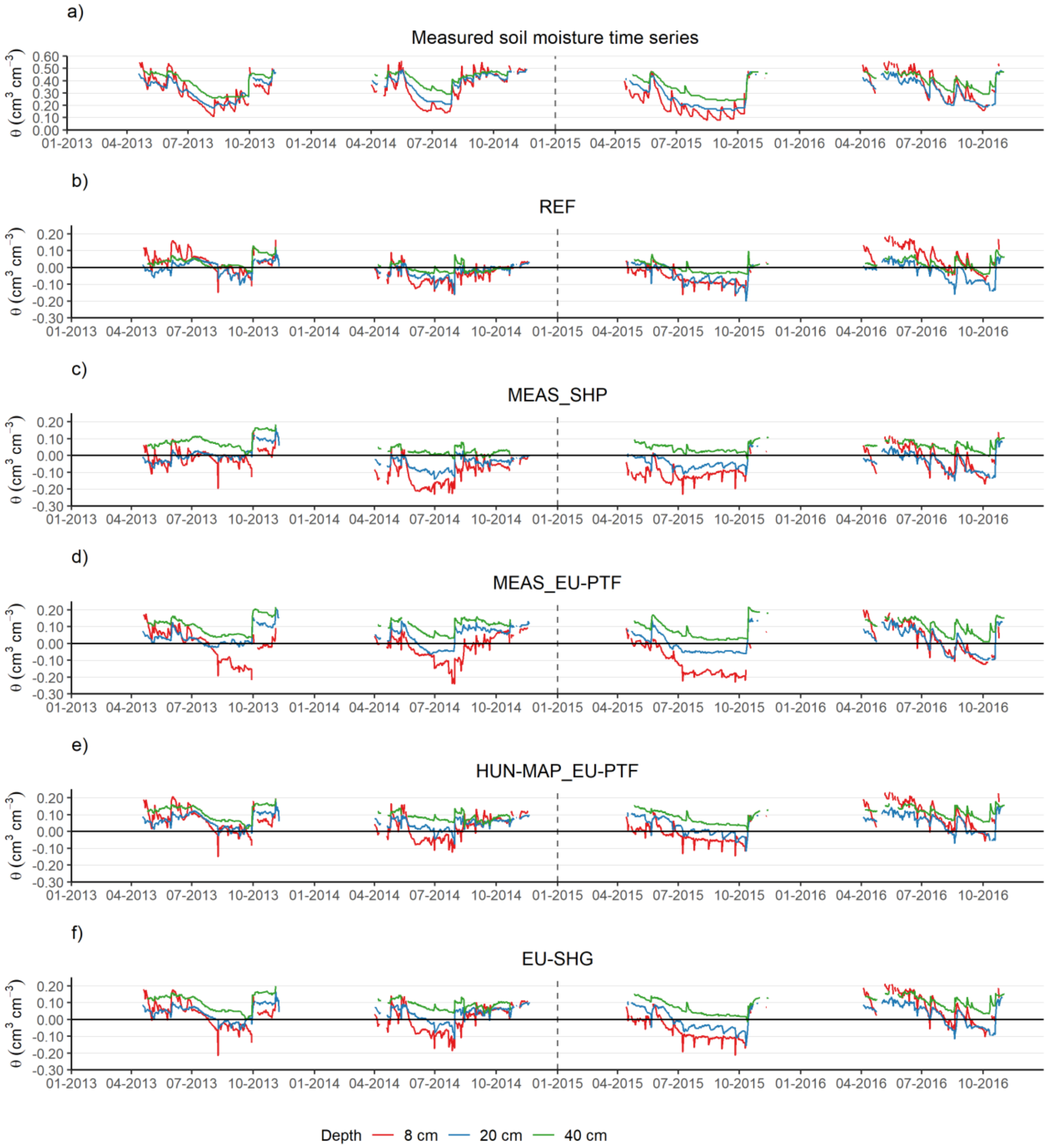

Figure 11. Residuals of the simulated soil moisture time series based on b) measured and c)-e) predicted soil hydraulic properties in relation to a) the observed soil moisture content for the Grassland Site.

2.4. Assessment of derived soil hydraulic parameters at catchamnet and profile scale

Catchment scale modelling

Both tested 3D datasets – the European and regional/national – were suitable for modelling the rainfall runoff processes of the Zala catchment in an adequate quality. The model performance of the two variants was satisfactory for the calibration and validation dataset of the Zalaapáti river gauge. The distribution of the water flow components is detailed and suitable for spotting dominant pathways across the watershed.

Model parameter calibration showed that soil hydrologic parameters are critical when hydrologic behaviour is to be studied. Available water content and saturated hydraulic conductivity were increased by the optimization algorithms for all soil classes (dominant soil classes were included in the calibration process only) and soil layers. There were no substantial differences between the two models regarding the spatial distribution of the water balance components.

These results lead to the conclusion that for the studied catchment the accuracy of the SWAT model could not be improved solely using more accurate soil dataset. This can be explained by the mechanism of SWAT model that is, it calculates hydrological processes on spatially aggregated units, hence it relies strongly on calibration. The newly derived soil hydraulic database should be tested in smaller scale applications with a more deterministic, fully distributed hydrologic model in order to highlight spatial differences of hydrological processes due to different soil data structures. However, this model experiment provides useful practical information, as SWAT and methodologically similar algorithms are more common than the highly complex, data- and calculation intensive fully distributed hydrological models.

Profile scale modelling

Major differences occurred in the simulated water budgets, which can be attributed to the different environmental conditions at the three sites. Water budget results are mostly in line with the model efficiency indicators: on-site measured soil hydraulic parameters led to different results from the others. Based on the presented results we can assume that the widely used soil profile description and sampling practice might not properly suit the input needs of hydraulic simulations and can increase the uncertainty of modelling. The performance of soil hydraulic parameters derived with pedotransfer functions is promising, we will continue the more detailed analysis of 3D soil hydraulic property maps.

According to the experiences of the modelling, the depth distribution of hydraulic conductivity is the most influencing factor for both model efficiency and water budget calculations. General low performance of the MEAS_SHP variants can be explained with the well-known high uncertainty of saturated hydraulic conductivity measurements. This points out that calibration of this parameter is inevitable in case of plot-scale soil hydrological studies, where the aim is the precise temporal description of soil moisture. However, the derived soil moisture retention curve parameters provide significant support for such a calibration process, as the number of optimised parameters are reduced greatly with their help (for each soil layer only the K_s has to be adjusted instead of θ_r, θ_s, α, n and K_s).

M3: The derived soil hydraulic maps of thw catchment of Lake Balaton are freely available from the website of the from the Institute for Soil Sciences and Agricultural Chemistry Centre for Agricultural Research:

- in GeoTIFF format: https://www.mta-taki.hu/en/kh124765/maps
- Online Map Viewer of the derived soil hydraulic maps: https://www.arcgis.com/home/webmap/viewer.html?webmap=88f7b66bd2d040758bf24f97958de210&extent=16.3392,46.3353,18.3675,47.1036

Project results used by other research activities

The derived 3D soil hydraulic dataset is used to assess the hydrological ecosystem services (KEHOP-4.3.0-15-2016-00001) (Decsi et al., 2020), comply functional soil maps (NKFI - K 131820) (Pásztor et al., 2020), model natural/small water retention measures (H2020 - 8627456 - OPTAIN) and provide information for sustainable water management (WaterJPI – iAqueduct) (Su et al., 2020). The soil hydraulic parameters were computed with the project's HUN-PTFs for the Biome-BGCMAg biogeochemical model (GINOP-2.3.2-15-2016-00028) (Fodor et al., 2020). The results of the soil profile descriptions were used in Molnár et al. (2019) to study correlations between soil properties.

Dissemination

We created the website of the project: http://mta-taki.hu/en/kutatasok/3d-talaj-vizgazdalkodasi-terkepkeszites-uj-modszertananak-kidolgozasa-es-alkalmazasanak (HU), http://mta-taki.hu/en/kh124765 (EN) for wider dissemination of the project results. The 3D soil hydraulic maps of the Balaton catchment – in GeoTIFF format – and the hydraulic pedotransfer functions – in RData format – are freely available for non-commercial use from the Institute for Soil Sciences and Agricultural Chemistry Centre for Agricultural Research (http://mta-taki.hu/en/kh124765/maps, last access: 24 February 2020, (Szabó et al., 2018b); https://www.mta-taki.hu/en/kh124765/hun_ptfs, last access: 24 February 2020, (Szabó et al., 2018a). The maps are accessible in GeoTIFF format and in an online map viewer.

The parametric PTFs are available from a user friendly web interface: https://ptfinterface.rissac.hu (Szabó et al., 2019c) both in Hungarian and English to facilitate their use.

We presented the MARTHA ver3.0 dataset in the Conference of Hungarian Soil Science Society (Tóth et al., 2018a) and published in Szabó et al. (2019a). The transfer functions for particle size data harmonization were published in Makó et al. (2017) and Makó et al. (2019).

The methodology of deriving PTFs has been published in Van Looy et al. (2017) and a book chapter (Rajkai et al., 2018) - in the book chapter there was no opportunity to acknowledge the project. The methodology of soil hydraulic mapping was presented in the AGU Fall Meeting (Tóth et al., 2017b). The new Hungarian point PTFs (HUN-PTFs), the mapping approaches and the 3D soil hydraulic dataset of the catchment of Lake Balaton were published in Szabó et al. (2019a) and presented in international conferences (Szatmári et al., 2019; Tóth et al., 2019b, 2019a). The manuscript on mapping soil hydraulic conductivity for the catchment of Lake Balaton is under preparation.

Deriving Hydrological Response Units based on the newly derived soil hydraulic maps were presented in national (Laborczi et al., 2019) and international (Pásztor et al., 2019) conferences.

The manuscript (Szabó et al., 2019b) including the parametric PTFs has been submitted to the Geoscientific Model Development journal, the preprint is available from: https://www.preprints.org/manuscript/202002.0425/v1.

The results of profile scale hydraulic simulations has been published (Kozma et al., 2019a) and presented in the Conference of Hungarian Soil Science Society (Kozma et al., 2018), the Wageningen Soil Conference 2019 (Kozma et al., 2019b) and a manuscript on it is under submission. The catchment scale analysis of soil hydraulic maps was presented in the International soil and water assessment tool conference (SWAT 2019) (Jolánkai et al., 2019) and a manuscript is under preparation.

The social benefits of the knowledge of soil hydraulic properties were published in Manfreda et al. (2018); Stankovics et al. (2018); Tóth et al. (2018c) and presented in EGU conference (Tóth et al., 2018b).

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