Evapotranspiration prediction for European forest sites does not improve with assimilation of in-situ soil water content data

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10 **Abstract.** Land surface models (LSM) are an important tool for advancing our knowledge of the Earth system. LSM are constantly improved to represent the various terrestrial processes in more detail. High quality data, freely available from various observation networks, are providing being used to improve the prediction of terrestrial states and fluxes of water and energy. To optimize LSM with observations, data assimilation methods and tools have been developed in the past decades. We apply the coupled Community Land Model version 5 (CLM5) and Parallel Data Assimilation Framework (PDAF) system (CLM5-PDAF) for thirteen forest field

15 sites throughout Europe covering different climate zones. The goal of this study is to assimilate in-situ soil moisture measurements into CLM5 to improve the modeled evapotranspiration fluxes. The modeled fluxes will be evaluated using the predicted evapotranspiration fluxes with eddy covariance (EC) systems. Most of the sites use point scale measurements from, however for three of the forest sites we use soil water content data from cosmic-ray neutron sensors, which have a measurement scale closer to the typical land surface model grid scale and EC footprint. Our results show that while data assimilation reduced the root-mean-

20 square error for soil water content on average by 56 to 64%, the root-mean-square error for the evapotranspiration estimation is increased by 4%. This finding indicates that state-of-the-art LSM such as CLM5 still suffer from uncertainties in the representation of soil hydrological processes in forests, e.g. deep root water uptake, or highly uncertain vegetation parameters.

1 Introduction

Land surface models (LSM) are important tools to improve our understanding of the Earth system. LSM cover a broad range of land

25 surface processes like the partitioning of incoming energy at the land surface, mass exchange between the land and atmosphere, hydrological, and ecological processes. They use sophisticated parameterizations and are constantly improved to achieve a more accurate representation of land surface processes, e.g. Arora et al. (2020) and references therein. However, there are still many sources of uncertainty introducing systematic biases in the LSM (e.g. initial conditions, atmospheric forcings, parameters, and parameterization. One approach to improve model predictions is to assimilate observational data. Improved estimates of

30 evapotranspiration (ET) by LSM is of main interest as ET is a major driver of climate and and weather, an important component of

the water and energy cycles, closely coupled to the carbon cycle through the photosynthesis process (Jung et al., 2011). Fine spatial scale ET estimations are important to estimate water use and plant stress (Wurster et al. 2020). The flux of ET is, however, influenced by multiple factors, including soil water content, soil properties, ecophysiological processes, and vegetation characteristics (Wilson et al., 2004), so it is more common to assimilate these prognostic variables rather than ET itself.

Many studies assimilate soil moisture products into LSMs (e.g. Hung et al., 2022; Mahmood et al., 2019; Naz et al., 2019; Liu and Mishra., 2017; Han et al., 2015) and report on the impact on hydrological variables like root-zone-moisture and runoff. Some studies use assimilation of soil water content or related variables to evaluate ET estimation of LSMs. For example, Girotto et al. (2017) assimilated terrestrial water storage from the Gravity Recovery and Climate Experiment into a land surface model and evaluated

40 results over India. However, they found that the assimilation decreased the accuracy of ET estimation compared to observations due to model limitations in representing irrigation. Peters-Lidard et al. (2011) assimilated two different remotely sensed soil water content products into the Noah land surface model over North America and found mixed results regarding the improvement of latent heat flux estimates . The domain averaged root-mean-square error of the latent heat flux reduced from 27.6 Wm⁻² to 25.6 Wm⁻² or increased to 29.4 Wm⁻² depending on the assimilated soil water content product. Additionally, they show that the improvements and

45 degradation vary spatially across their study domain, with land cover type, and as function of the season and they note that the most significant improvements occur for cropland and grassland. Liu and Mishra (2017) assimilated surface soil water content data from the Advanced Microwave Scanning Radiometer-Earth Observing System in a global Community Land Model version 4.5 and found ET bias reductions of up to 2.5mm/day compared to the Global Land Data Assimilation System (GLDAS) data product.

50 For our study, we chose the latest version (version 5) of the widely used Community Land Model (CLM5) (Lawrence et al. 2019) as various land surface process representations have been improved in CLM5 compared to earlier versions. For instance, Kennedy et al. (2019) added a plant hydraulic stress parameterization to improve the accuracy of simulated transpiration and soil water content. Lawrence et al. (2019) demonstrated the improvements of CLM5 over its precursor CLM4 in terms of ET using two study sites as examples and highlighted the better representation of the effects of soil depth on ET prediction in CLM5. On the other hand, Cheng

55 et al. (2021) found that CLM5 predicts lower ET compared to older CLM versions and various observational data, likely due to low photosynthetic rate and leaf area index (LAI), which is consistent with their finding of low gross primary production (GPP) compared to reference data in the same simulations. In addition to these regional to global validation studies, CLM was used in several single point setups, i.e. simulations for a single grid cell, to evaluate the performance of various LSM components. For example, Hudiburg et al. (2013) used CLM 4.0 to estimate net primary production (NPP) and GPP of a forested site and compared it with eddy covariance

60 (EC) measurements. Another study (Zhang et al., 2019) reduced an overestimation of growing-season LAI and annual GPP of a grassland site for a CLM 4.5 single-point setup. More recently, CLM5 was extended to consider both cover crop management with improvements to ET estimation of up to 57% (Boas et al., 2021) and fruit tree cultivation using extensive field measurements with high correlation between observed and modeled ET (Dombrowski et al., 2022).

65 In this study, we investigate if assimilating high quality, in-situ soil water content measurements can improve the evapotranspiration estimates of LSM. We focus on one specific land cover type, namely forests. To investigate this, we use point and plot scale in-situ

soil water content measurements. For most sites we use point measurements provided by FLUXNET (Baldocchi et al., 2020) and eLTER Europe. The FLUXNET data have been used in various studies to verify or compare model results. For example, Dirmeyer et al. (2018) used FLUXNET data to compare four model systems, including CLM4.5, in three configurations and found for annual averaged ET that correlations range from 0.28 to 0.43 and for sensible heat from 0.14 to 0.54. The point scale measurements use invasive equipment and the specific measurement volume, exact depth of the sensors, number of sensors, and number of stations varies from site to site. For a few sites we use soil water content measurements from Cosmic Ray Neutron Sensing (CRNS) from the COSMOS-Europe data set (Bogena et al., 2022). The CRNS provides continuous and non-invasive soil water content measurements over a spatial footprint of hundreds-of-meters and integrates from the surface to a depth of 10-70 cm vertically in the soil (Zreda et al., 2008; Köhli et al., 2015). The spatial footprint area is similar to the footprint of the EC flux tower. We use the final processed data on soil water content and vertical penetration (measurement) depth provided by the COSMOS-Europe dataset (Bogena and Ney, 2021). In this study, we use the ensemble Kalman filter to assimilate in-situ soil water content measurements into CLM5 simulations and the effect on the modeling results are quantified by comparing the modeled ET against the observed ET obtained from EC flux towers. We also analyze the effects on other land-atmosphere exchange fluxes, i.e. net ecosystem exchange (NEE) and gross primary production (GPP). The paper is structured as follows: First, we introduce the model and data assimilation framework used. The sites selected for this study and the observational data used for data assimilation and model-observation comparison are then described. Subsequently, the results for each variable of interest are shown and analyzed. Finally, we end with a discussion of the obtained results and conclusions.

2. Methods and Materials

2.1 Study sites

In our study, we are interested in the characterization of water, energy and carbon exchange between (European) forest ecosystems and the atmosphere, and whether soil water content assimilation can improve the characterization of these processes. Therefore, we selected European sites with different forest types (see Table 1) covering different climate zones in Europe. Another important constraint was the availability of soil water content data and evapotranspiration measurements for the period from 2009 to 2018. The selected sites are mostly part of FLUXNET (Baldocchi et al., 2020) or the European Long-Term Ecological Research network (eLTER-Europe) (Parr et al., 2002). In addition to the sites from these observation networks, we included three sites from the COSMOS-Europe network (Bogena et al., 2022) where cosmic-ray neutron sensors (CRNSs) are installed to estimate the soil water content of the forested sites. Table 1 gives an overview of all selected sites for this study and Figure 1 shows the distribution on the map.

In this study, daily average soil water content data are assimilated and the model is verified using daily average evapotranspiration and sensible heat flux data. Since the observational data were already quality controlled by the providers, we did not filter out any

data. Additionally, gaps in soil water content observations were not filled and only soil water content data were assimilated for days

100   when observations were available. Similarly, simulated evapotranspiration was only compared with observations when data were

available.

2.2 Model description

For our study, we used the Community Land Model version 5.0 (CLM5) that can be applied in various configurations (Lawrence et

105   al. 2019). We use CLM5-BGC, i.e. CLM5 with the biogeochemistry module active as opposed to CLM5 with fixed phenology. The

biogeochemistry module enables a fully prognostic treatment for carbon and nitrogen in the land surface model and has a significant

impact on the modeled water and energy budgets.

CLM5 uses a sub-grid hierarchy of various Plant Functional Types (PFTs) to characterize the land-use and vegetation type within

110   every grid cell, e.g. evergreen needle leaf or deciduous broad leaf forests. CLM5 contains a spatially variable soil depth with an

underlying, impermeable bedrock instead of the unconfined aquifer parameterization used in the former CLM4 versions. To estimate

the soil water content, CLM5 solves the Richard's equation using the Brooks-Corey parameters derived from pedotransfer functions

from Clapp and Hornberger (1978) with a finite-difference approximation to represent the vertical discretization and temporal

evolution of soil water content.

115   The sensible and latent heat flux estimation in CLM5 is derived from the Monin-Obukhov Similarity Theory and differentiated for

vegetated and non-vegetated surfaces. We only study forested areas where CLM5 partitions the sensible heat and latent heat flux into

vegetation and ground fluxes. For the vegetation part the contributions from the leaf boundary layer, the sunlit and shaded stomatal

resistances affect the total resistance to the modeled water vapor transfer. The water vapor transfer includes transpiration from dry

leaf surfaces and the transpiration removes water from the soil based on root fraction for a given soil layer. Interception, throughfall

120   and canopy drip are explicitly modeled in CLM5 and canopy evaporation is partitioned from stem and leaf surface evaporation based

on the vegetation temperature. The ground fluxes, e.g. from bare soils or soil beneath a canopy, are dependent on the ground surface

temperature. The ground latent heat flux is reduced if not enough soil moisture is available and the excess energy is redistributed to

the sensible heat flux. The detailed procedure and equations are documented in Lawrence et al. (2018).

2.3 Data assimilation

2.3.1 Ensemble Kalman filter

In this work, assimilation of soil water content measurements is performed with the Ensemble Kalman Filter (EnKF) (Evensen, 1994; Burgers et al., 1998). The EnKF uses an ensemble modeling approach, with various simultaneous model runs, to approximate the model uncertainty. The ensemble members have different input model parameters and atmospheric forcings (see section 2.4 for details). We define a state vector x and an observation vector y, e.g.

$$\mathbf{x}^i = \begin{pmatrix} \theta^i_{1,1} \\ \theta^i_{1,2} \\ \cdots \\ \theta^i_{1,m} \\ \cdots \\ \theta^i_{n,m} \end{pmatrix} \quad (1)$$

where n is the number of layers and m is the number of grid cells, $\theta^i_{j,l}$ is the soil water content for layer j and grid cell l of the model and the superscript i refers to ensemble member i.

$$\mathbf{y} = \mathbf{o} + \mathbf{e} \quad (2)$$

where o is a vector of the observational data and e represents a perturbation vector with mean zero and covariance according to the observational error covariance matrix. This perturbation vector is used to correct the error statistics as described in Burgers et al. (1998).

The update step of the ensemble Kalman filter is:

$$\mathbf{x}^i_a = \mathbf{x}^i_f + \mathbf{K}\left[\mathbf{y} - \mathbf{H}\mathbf{x}^i_f\right] \quad (3)$$

where the superscript i refers to ensemble member i, $\mathbf{x}^i_a$ is the updated state vector after the analysis, $\mathbf{x}^i_f$ is the forecasted model state vector, K is the Kalman gain and H is the measurement operator that transforms between model and observational states. In this study, the measurement operator H consists of a simple mapping of the observations to the corresponding model layers in the state vector for simulations with point measurements. For simulations assimilating CRNS, H assigns the mean observed SWC to all the layers down to the measurement depth. This is a simplified approach and will be improved in further studies to take the weighting function from Schrön et al. (2017) into account. The Kalman gain is calculated accordingly:

$$\mathbf{K} = \mathbf{P}\mathbf{H}^T(\mathbf{R} + \mathbf{H}\mathbf{P}\mathbf{H}^T)^{-1} \quad (4)$$

where the superscript T is used for transposed matrices, P is the model error covariance matrix, which is approximated through ensemble statistics, specifically:

$$P = \frac{1}{(N-1)} \sum_{i=1}^{N} \left(\mathbf{x}_f^i - \overline{\mathbf{x}_f}\right)\left(\mathbf{x}_f^i - \overline{\mathbf{x}_f}\right)^T \quad (5)$$

150   where N is the number of ensemble members and $\bar{x}$ is the ensemble mean.

In this study, the state vector depends on the simulation scenario (explained in more detail in section 2.3.2).

To enable data assimilation with CLM5, we use the Parallel Data Assimilation framework (PDAF) (Nerger et al. 2005), which was recently coupled to CLM5 (Strebel et al. 2022). This coupling (CLM5-PDAF) also supports the assimilation of soil water content measurements.

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2.3.2 Parameter updating

In addition to the use of data assimilation for state updating, we also perform parameter updating based on the state augmentation approach (Friedland, 1969; Fertig et al., 2009). Here, model parameters are attached to the state vector and updated based on the Kalman gain calculations without observations of the model parameters. By default, CLM5-PDAF updates soil hydraulic parameters

160   through changes to fractions of sand, clay, and organic matter and the pedotransfer function of Clapp and Hornberger (1978). In this indirect approach the state vector for the EnKF is defined as follows:

$$\mathbf{x}^i = \begin{pmatrix} \theta^i \\ \%sand^i \\ \%clay^i \\ \%organic^i \end{pmatrix} \quad (6)$$

where the superscript i refers to ensemble member i. The components θ, %sand, %clay, and %organic each represent a vector containing the respective variable for each soil layer of each grid cell of the model.

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2.4 Model setup

2.4.1 Domain setup

Since we only use local field measurements, we represent each study site as a single grid cell in CLM5. This approach is also consistent from the viewpoint of larger regional scale models, where each of these sites would only be part of a grid cell. The CLM5

170   grid cells are vertically divided into 25 layers from the surface down to 50 m depth of which the first 20 layers (until 8.6 m depth)

may be hydrologically and biogeochemically active depending on the variable soil depth for each site (Lawrence et al., 2018). For

the more than 70 different surface parameters of CLM5, we used the default values generated by the tools provided with CLM5 (e.g.

soil depth to bedrock, sand, clay, and organic matter fractions, PFTs). These default values are generated from remapping various

global files (Lawrence et al., 2019). Only the PFT were manually assigned for each site. For the ensemble creation, the fractions of

175   sand, clay, and organic matter are modified for each ensemble member. The perturbations are normally distributed with mean zero

and a standard deviation of 10%. For FLUXNET sites, measured soil water content is provided for up to three depths described as

superficial, medium, and deep. Since data assimilation in CLM5-PDAF requires a specific vertical layer, we assigned 5, 20 and 50

cm to the respective FLUXNET SWC layers. For the CRNS sites, the measurement depth for each individual measurement is

calculated following Schrön et al. (2017) and is included in the dataset from Bogena et al. (2022).

2.4.2 Atmospheric forcings

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Meteorological observations were also available at the selected study sites and were used to force CLM5. The existing gaps in the

observation time series were gap-filled with data from the COSMO-REA6 reanalysis data product (Bollmeyer et al., 2015). For the

ensemble generation precipitation (PR), shortwave radiation (SW), longwave radiation (LW), and air temperature (TA) were

perturbed taking into account cross-correlations between variables according Reichle et al. (2007). The perturbations are:

185   multiplicative PR ~ logN(1, 0.5), multiplicative SW ~ logN(1, 0.3), additive LW ~ N(0, 20) (W/m2), and additive TA ~ N(0, 1) (°K).

The following cross-correlation coefficients between variables were used: PR–SW -0.8, PR-LW 0.5, PR-TA 0, SW-LW -0.5, SW-

TA 0.4 and LW-TA 0.4.

2.4.3 Data assimilation experimental setups

Three different simulation scenarios were considered: 1) Open loop (OL) simulations without data assimilation; 2) Data assimilation

190   with updating of soil water content (DAS); and 3) Data assimilation with soil water content updating and parameter updating (DASP).

For all scenarios data assimilation is performed at a daily frequency and with daily averages from the observations. For DASP a

damping factor of 0.1 is used on the parameter updates to avoid filter inbreeding and keep the ensemble spread larger so that the

model error covariance matrix is a good approximation for model uncertainty.

2.5 Statistical metrics

195 For the comparison of simulation results with observations, we use four statistical metrics: the squared correlation coefficient (R^2),

the mean bias error (MBE), the root-mean-square error (RMSE), and the unbiased root-mean-square-error (ubRMSE):

$$R^2 = 1 - \frac{\sum_{t=1}^{Nt}(o^t - m^t)^2}{\sum_{t=1}^{N}(o^t - \overline{o^t})^2} \quad (7)$$

$$MBE = \frac{\sum_{t=1}^{Nt}(m^t - o^t)}{Nt} \quad (8)$$

$$RMSE = \sqrt{\frac{\sum_{t=1}^{Nt}(m^t - o^t)^2}{Nt}} \quad (9)$$

200 $$ubRMSE = \sqrt{\frac{\sum_{t=1}^{Nt}\left[(m^t - \overline{m^t}) - (o^t - \overline{o^t})\right]^2}{Nt}} \quad (10)$$

where o stands for observations, m represents the ensemble average of the simulated values, t is the time step, Nt the total number of

time steps and overbar represents the average over all time steps.

3. Results

205 ### 3.1 Soil water content

Figures 2, 3 and 4 show the results of the soil water content simulations at 20 cm depth of the OL, DAS and DASP simulations

compared to the soil water content observed at the nine sites. The corresponding scatter diagrams for the depths 5 and 50 cm can be

found in the appendix (Figures A1, A2, A3, and A4). Overall, the results show expected improvements by data assimilation of

observed soil water content. For the OL simulations, Fig. 2 shows particularly large RMSE values for CZ-BK, DE-Obe, FI-Sod and

210 NL-Loo. Fig. 3 illustrates the improved performance achieved by DASP, with a RMSE reduction from 29.3 cm³/cm³ to 6.25 cm³/cm³

and a MBE reduction from 28.06 cm³/cm³ to -2.94 cm³/cm³ for FI-Sod. Parameter updating, as shown in Fig. 4, further improves the

simulation results, but the improvement from DAS to DASP is significantly less than from OL to DAS.

The results of the three COSMOS-Europe sites are shown in Figure 5, in which the observed SWC values are compared with the

weighted SWC mean of the model layers corresponding to the measurement depth of CRNS. This comparison again shows the large

215 improvement from OL to DAS, and a smaller improvement or even a small deterioration from DAS to DASP.

3.2 Evapotranspiration

The impact of the data assimilation on the ET flux is shown in Figures 6 and 7. Notably, the difference between the OL and the DASP results is smaller for ET than for SWC. While the data assimilation improves the model results for SWC for all sites, both improvement and deterioration occur for modeled ET. Figure 8 shows the comparison of the improvements by data assimilation for SWC and the positive and negative effect on ET estimation. The average RMSE reduction for the DASP SWC prediction is between 56% and 64% compared to OL. Comparing the OL and DASP results for ET shows an average reduction of the MBE of 0.06 mm/day, but an increase in RMSE for the DASP ET predictions of 4 % on average, with 8 of the 13 sites showing a relative change in ET of only +/- 1 %. Two outliers (FI-Sod and NL-Loo sites) reduce the average model improvement in particular. These sites show both a large overestimation in SWC in the OL (see Fig. 2) and a large underestimation of ET in the DASP simulation (see Fig. 7). This indicates that the SWC-ET relation is incorrect for these sites. A possible explanation is the water uptake by roots in the deeper layers is underestimated for forest sites, as also suggested by Shrestha et al. (2018). Fig. 8 shows that the quality of the model results is not dependent on the forest type, i.e. the evergreen needle leaf forests (ENF) sites show both strong and average relative changes in SWC RMSE and ET RMSE. This suggests that the strong deviations in the model results of the FI-Sod and NL-Loo sites are due to other local conditions, e.g. soil properties.

The three CRNS sites show an average relative change of ET RMSE of -2.6%, -0.2%, and -0.9% for DE-HoH, DE-Wue, and DK-Glu, respectively. Therefore, although the CNRS measurements are more consistent with the large measurement area of the flux towers, no significant improvement in ET for these three sites can be achieved with the current implementation of the CNRS-SWC assimilation. We anticipate that the implementation of a more accurate observation operator would improve the modeled SWC. The current observation operator does not use vertical weighting to take the decreasing CRNS sensitivity with depth into account.

3.3. Evaluation of other land-atmosphere exchange fluxes

Comparing measured and modeled sensible heat fluxes (SH) are compared to measurements (Figures 9 and 10), similar R² values are obtained for the OL and the DASP approach. The R² values range from 0.23 to 0.51 with an average of 0.36. This is similar to the

ET results, where the R² of measured and modeled (OL and DASP) ET range from 0.01 to 0.58 with an average of 0.37. Comparing Fig. 9 and Fig. 10 shows the impact of data assimilation of SWC on SH to be small. On average DASP improves the MBE by 4.66 W/m² compared to OL. However, for five of the eight sites the improvement of the MBE is smaller than 1 W/m². But, compared to the ET results data assimilation of SWC reduces the MBE of SH for all sites.

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The impact of updating SWC with data assimilation on modeled Nee, GPP, and LAI is shown in Fig. 11. The NEE is negative (land acts as carbon sink) for eight, seven, and six of the field sites for OL, DAS, and DASP respectively. For DASP the GPP and LAI show an increase for two of the sites, a decrease for three of the sites and remain similar for eight of the sites. Fig. 12 shows how average SWC in 5 cm and 50 cm depth, ET, NEE, GPP and SH (average over all sites and all years) are affected by data assimilation.

250 Although DASP adjusts SWC at 5cm towards the observations, the correction for SWC at 50cm depth is smaller because not all sites provide data at this depth. In spite of improved SWC characterization, ET deviates slightly more from the observations after DASP, while sensible heat flux is very slightly closer to the observations. GPP is lower after DASP and NEE less negative. While the overall change for some of these variables is small, different variations throughout the year can be observed. This averaging hides the variations between sites and annual variability but highlights the overall model behavior. Notably, the data assimilation improves

255 SWC estimation at 5cm throughout the year while at 50 cm depth the improvement can mainly be observed in late summer and autumn. Similarly, for SH a model structural bias is apparent with large negative simulated SH values in late autumn, winter, and early spring while the observations show only a few days with negative average values over all sites and all years.

4. Discussion

4.1 Soil water content improvements

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Our results confirm that assimilation of high quality in-situ SWC data improves the prediction of SWC by CLM5, as it has been demonstrated in several other studies (Hung et al., 2022; Mahmood et al., 2019; Naz et al., 2019; Liu and Mishra, 2017; Han et al., 2015). In our study, we were able to show that this also applies to forest sites with different climates, tree species, and soil properties. Additionally, CRNS observations represent SWC for a larger area in better correspondence to the EC tower footprint. So far, only

265 few studies have used CRNS information in a data assimilation framework (Rosolem et al., 2014; Han et al., 2015; Baatz et al., 2017, Patil et al., 2021). In line with our study, these studies show the high potential of CRNS for improved soil moisture prediction with land surface models, both in terms of SWC prediction as well as in improving soil hydraulic parameters. Currently, CRNS stations are operated with increasing numbers worldwide (Andreasen et al., 2017), in hydrological observatories (e.g. Bogena et al., 2018; Lui et al., 2018), as national networks (Zreda et al., 2012; Evans et al., 2016) or even increasing at continental scales (e.g. Hawdon

270 et al., 2014; Bogena et al., 2022), which opens up new opportunities for assimilation of CRNS data in land surface models at various scales.

In our data assimilation approach, we assumed that the CRNS signal shows a constant sensitivity to SWC down to the penetration depth of the CRNS. However, Schrön et al. (2017) have shown that the integrated neutron signal over a vertical soil column exhibits a strong decrease in sensitivity with depth and suggested that this physical behavior of neutrons should be taken into account in model

275 applications. For example, Shuttleworth et al. (2013) developed a simple, physically-based analytical model to translate model-predicted soil moisture profiles into aboveground fast neutron counts within a data assimilation framework. A simpler method was proposed by Schrön et al. (2017) by using vertical weighting functions that depend on SWC, atmospheric pressure, horizontal distance and vegetation height. Therefore, in a follow-up study, we will test whether observation operators that account for the vertical weights of the different model soil layers according to the decreasing sensitivity of CRNS with depth will improve our SWC prediction

280 results.

4.2 Evapotranspiration estimation without improvements from SWC DA

Several studies have demonstrated the potential of improved ET prediction using data assimilation of SWC measurements (Liu and Mishra, 2017; Girotto et al., 2017; Lidard et al., 2011). These studies focused on regional or global scale and show heterogeneous

spatial patterns of improvement to ET estimation. Baatz et al. (2017) showed that assimilation of CRNS observations altered the ET

285   estimation in CLM4.5 in parts of their study area by up to 80 mm per year compared to the OL approach.

However, in our study with the land surface model CLM5 that data assimilation of SWC does not improve the ET prediction for

European forest sites. We also found that the impact on ET from assimilating CRNS observations is similarly limited as assimilation

of other in-situ SWC data Since our study sites cover a variety of climates and soil types, we assume that this result also applies to

other forest sites worldwide with similar tree species.

290   The lack of improvement in ET prediction in the case of data assimilation of in-situ soil moisture information is consistent with

findings from other studies. Girotto et al. (2017) found a decrease in ET accuracy after assimilating GRACE data over India and

attributed the results to the representation of irrigation in the model. Similarly, Peters-Lidard et al. (2011) showed mixed results after

assimilating multiple satellite soil water content products over North America with spatial variation of improvements and

deterioration of ET estimation. Overall, for 9 of the 13 forested study sites our OL simulations show positive mean bias error

295   indicating that CLM5 underestimates the ET compared to the FLUXNET observations. These underestimations are in agreement

with the results shown in the study by Cheng et al. (2021) showing that CLM5 underestimates ET observations. Additionally, Nearing

et al. (2018) investigated the contribution of model structural errors and model inputs for four different LSM and concluded that

SWC uncertainty was dominated by soil parameter uncertainty while ET uncertainty was dominated by forcing uncertainty. Without

a similar in-depth benchmark study for CLM5, but from our results and the results of the previously mentioned CLM5 studies a

300   similar conclusion can be drawn for CLM5.

A different aspect is that we assume that the EC data are correct to validate our simulation results. However, the EC-data might be

affected by energy balance closure issues (Foken, 2008; Hendricks Franssen et al., 2010).

4.4 Methods to improve ET estimation

There are various approaches to improve modeled ET estimates. For example, Zhang et al. (2020) identified and optimized four

305   hydraulic and three vegetation parameters in CLM4.0 that improved ET estimation by 7.3% for the optimization period and 5.3% for

the validation period for China. Similarly, Post et al., (2017) calibrated eight parameters to improve NEE estimation in CLM 4.5 and

a similar approach to optimize vegetation parameters in CLM 5.0 for ET estimation could improve simulation results. Tang et al.

(2015) implemented a root hydraulic redistribution model in CLM4.5 to improve ET estimation but found that their method was only

able to improve ET predictions north of 20°N. They identified the representation of deep roots, soil hydraulic parameterization for

310 certain soils, meteorological forcings, and the parameterization of the water table dynamics and drainage as the main limitations to improve ET by their method.

Denager et al. (2022) used SWC measurements for an agricultural site in Denmark for parameter calibration of soil texture, LAI, stomata conductance and the root distribution in CLM5 and obtained improved energy partitioning of ET and SH. However, they also found it difficult to calibrate the parameters to get an improvement in SH estimation throughout the year and suggested that the

315 difference in energy balance closure between LSMs and EC flux observations contributes to the bias.

Fox et al. (2022) concluded that errors in LAI estimations in LSMs lead to substantial flaws in the representation of carbon, water, and energy fluxes. Furthermore, they conclude that data assimilation to remove bias in LAI improves LSMs results significantly and is advisable until the prognostically modeled LAI improves substantially. For example, Zhang et al. (2016) assimilated remotely sensed LAI data into the Biome-BGC model at two sites and improved both ET and NEE estimates, evaluated with EC tower

320 measurements. Rahman et al. (2022) showed that the joint LAI and topsoil SWC assimilation from satellite products improved the ET estimation for the Contiguous United States compared with independent validation datasets. While data assimilation of topsoil SWC alone only improved the SWC estimation.

As mentioned, LAI is identified as a key variable to improve ET estimation and representation of land carbon processes. Therefore, in future work we will investigate the effects of data assimilation of LAI and joint state-vegetation parameter estimation on the

325 simulation of carbon, water, and energy fluxes with CLM5.

5. Conclusions

This paper analyzed the impact of the assimilation of in situ soil water content (SWC) data on SWC characterization, evapotranspiration (ET), sensible heat flux (SH), gross primary production (GPP) and net ecosystem exchange (NEE), for 13 forested sites in Europe. Assimilation of SWC, from both point scale and plot scale observations, with the Ensemble Kalman Filter, using the Community Land Model version 5 coupled to the Parallel Data Assimilation Framework (CLM5-PDAF) improves SWC prediction (RMSE reductions between 56% and 64% compared to the open loop run, and depending on measurement depth). However, assimilation of in situ SWC does not improve the ET prediction for the investigated European forest sites. For most of the sites, data assimilation showed almost no effect on ET fluxes (RMSE changes between +/- 1%) and some sites showed strong negative effects of SWC assimilation on ET predictions (-20% to -30% change in RMSE). The assimilation of in situ SWC from Cosmic Ray Neutron Sensors (CRNS), which determine SWC over a larger horizontal footprint more in correspondence with the eddy covariance footprint, for three of the 13 sites, also does not improve ET characterization. These results suggest that state-of-the-art LSM such as CLM5 still suffer from uncertainties in the representation of soil hydrological processes in forests, e.g. deep root water uptake, uncertainties in the representation of biological processes of tree transpiration, partly related to uncertain vegetation parameters. In the future, to improve modeled ET using data assimilation we will further examine the potential of assimilating different state variables, like for example leaf area index and updating related vegetation parameters. In addition, we will apply a measurement operator in the data assimilation framework that considers the vertical sensitivity of the CRNS signal

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Tables

525 **Table 1**: Overview of the study sites. Classification uses the International Geosphere-Biosphere Program Code (IGBP) as is used for FLUXNET: MF for mixed forests, ENF for evergreen needle leaf forests, DBF for deciduous broad leaf forests, EBF for evergreen broad leaf forests, WSA for woody savannah. LON is longitude and LAT latitude.

Site name	Country	Abbreviation	Code	LON	LAT	Data source	Mean annual temperature [°C]	Mean annual precipitation [mm]	Typical tree species
Brasschaat	Belgium	BE-Bra	MF	4.51	51.30	FLUXNET	9.8	750	Scots pine
Bílý Kříž forest	Czech Republic	CZ-BK	ENF	18.53	49.50	FLUXNET	7	1316	Norway spruce
Hainich	Germany	DE-Hai	DBF	10.45	51.07	FLUXNET	8.3	720	Mixed Beech
Hohes Holz	Germany	DE-HoH	DBF	11.21	52.08	COSMOS Europe	10	820	Mixed beech
Oberbärenburg	Germany	DE-Obe	ENF	13.72	50.78	FLUXNET	5.5	996	Norway spruce
Wüstebach	Germany	DE-Wue	ENF	6.33	50.50	COSMOS Europe	7	1180	Spruce
Gludsted	Denmark	DK-Glu	ENF	9.33	56.07	COSMOS Europe	8.2	1080	Spruce
Conde	Spain	ES-Cnd	WSA	-3.22	37.91	FLUXNET	15.8	474	Olive grove
Hyytiälä	Finland	FI-Hyy	ENF	24.29	61.84	LTER Europe	3.8	709	Boreal Scots pine
Sodankylä	Finland	FI-Sod	ENF	26.63	67.36	FLUXNET	-1	500	Boreal Scots pine
Puéchabon	France	FR-Pue	EBF	3.59	43.69	FLUXNET	13.5	883	Evergreen oak
Lavarone	Italy	IT-Lav	ENF	11.28	45.95	FLUXNET	7.8	1291	Coniferous forest
Loobos	Netherlands	NL-Loo	ENF	5.74	52.16	FLUXNET	9.8	786	Scots pine

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Figures
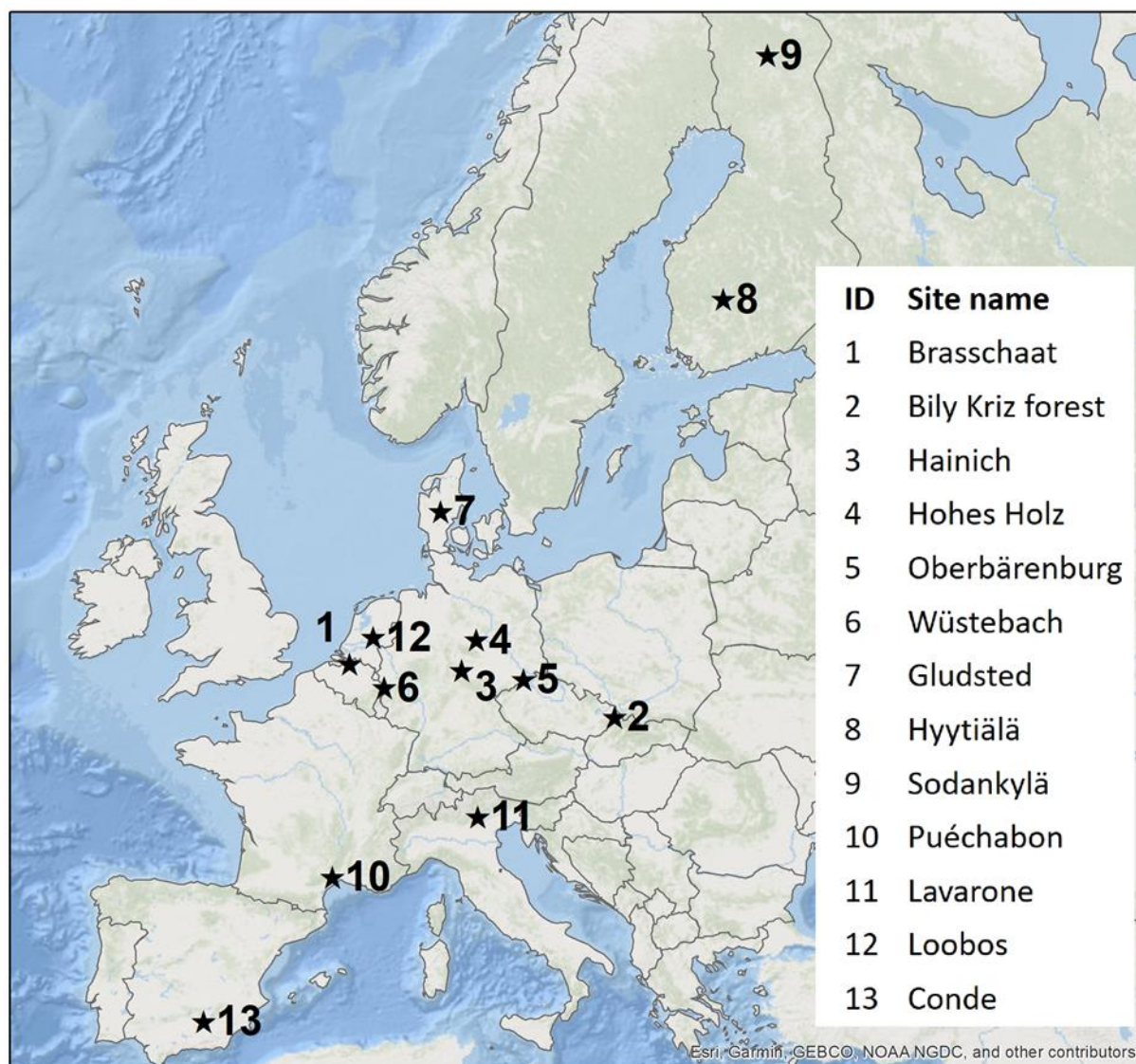
Figure 1: Map showing the location of the selected study sites of the FLUXNET, eLTER and COSMOS-Europe networks.

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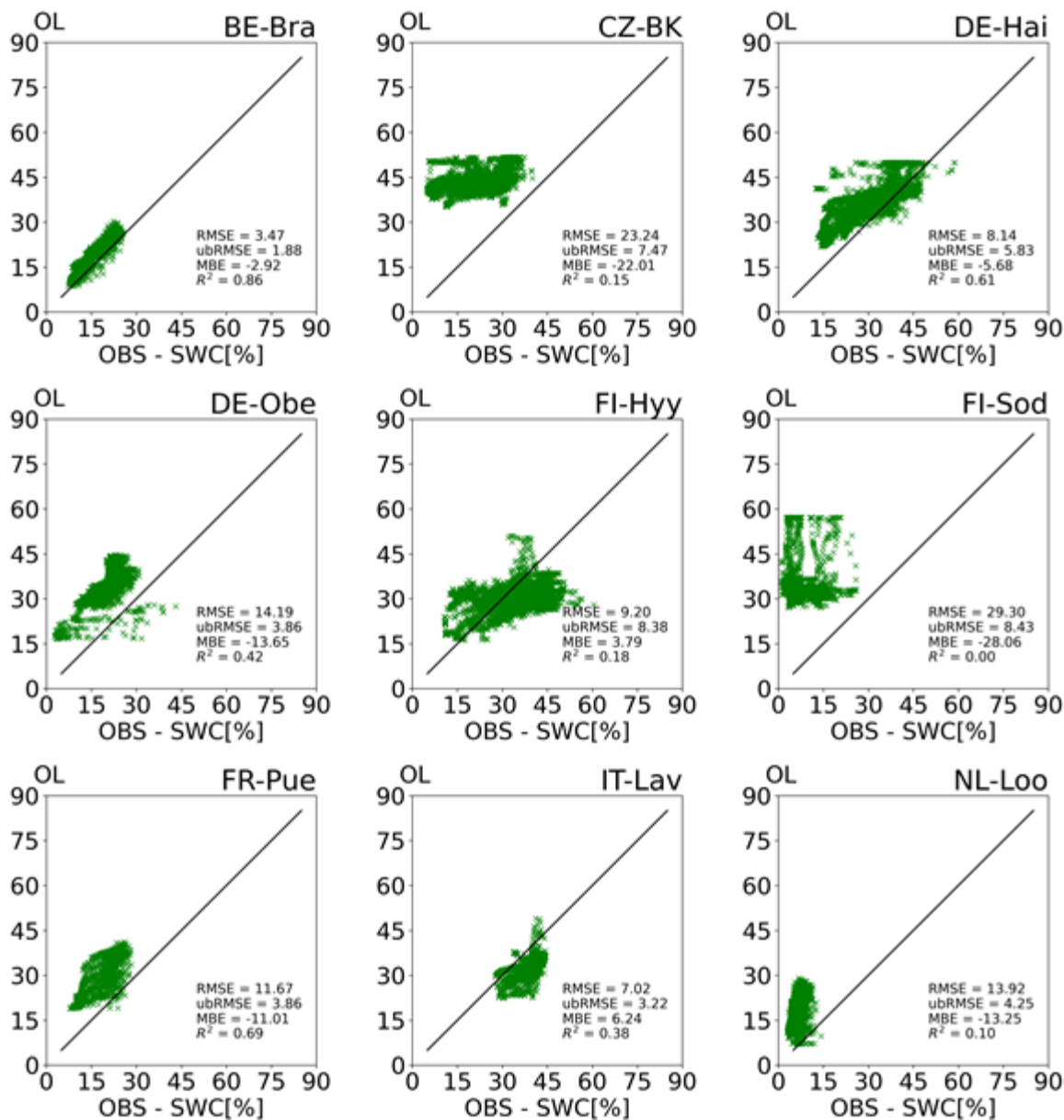


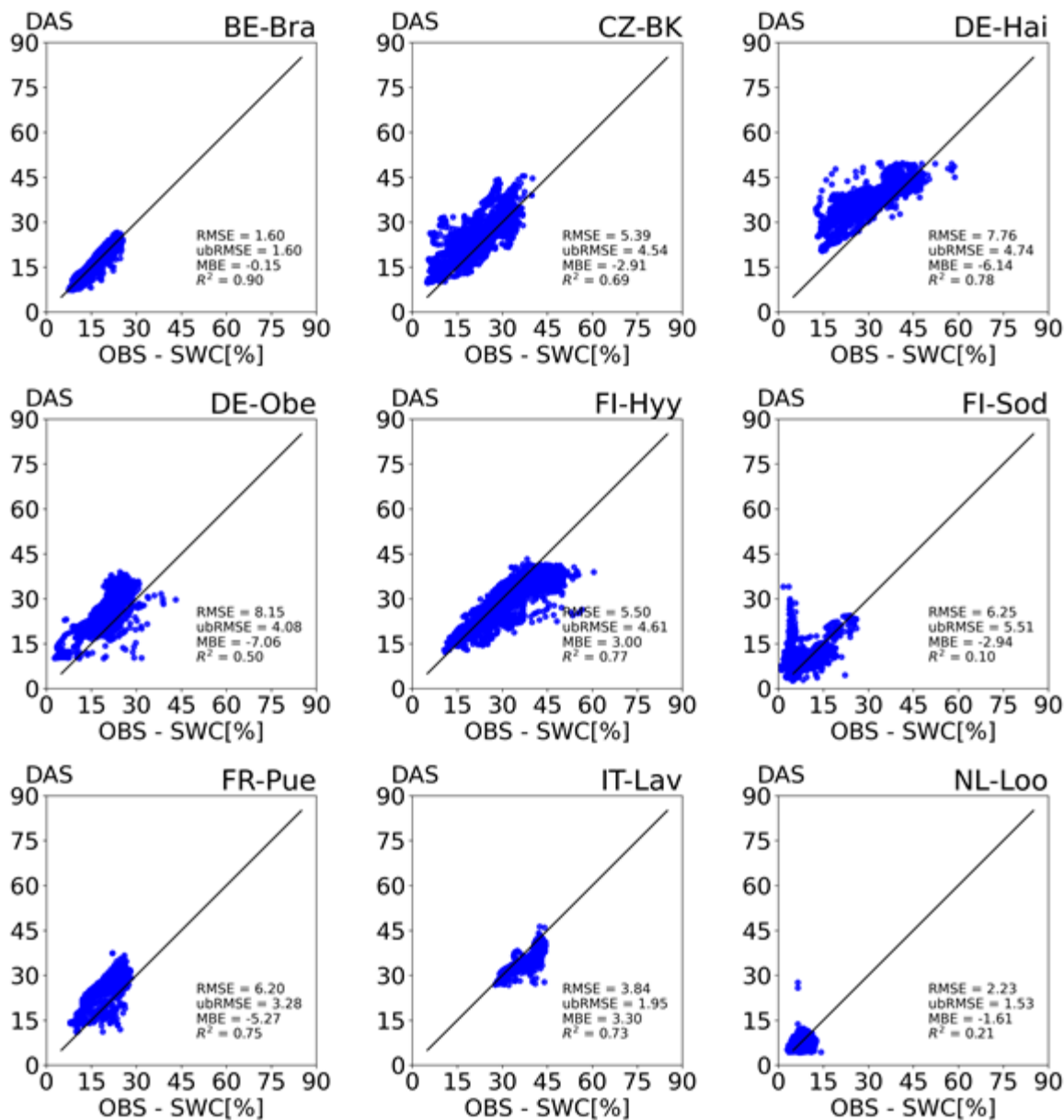
Figure 2: Scatter plots of observed soil water content at nine study sites versus OL simulation results at 20 cm depth. The points represent daily averages for the days observation data are available.

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Figure 3: Scatter plots of observed soil water content at nine study sites versus DAS simulation results at 20 cm depth. The points represent daily averages for the days observation data are available.

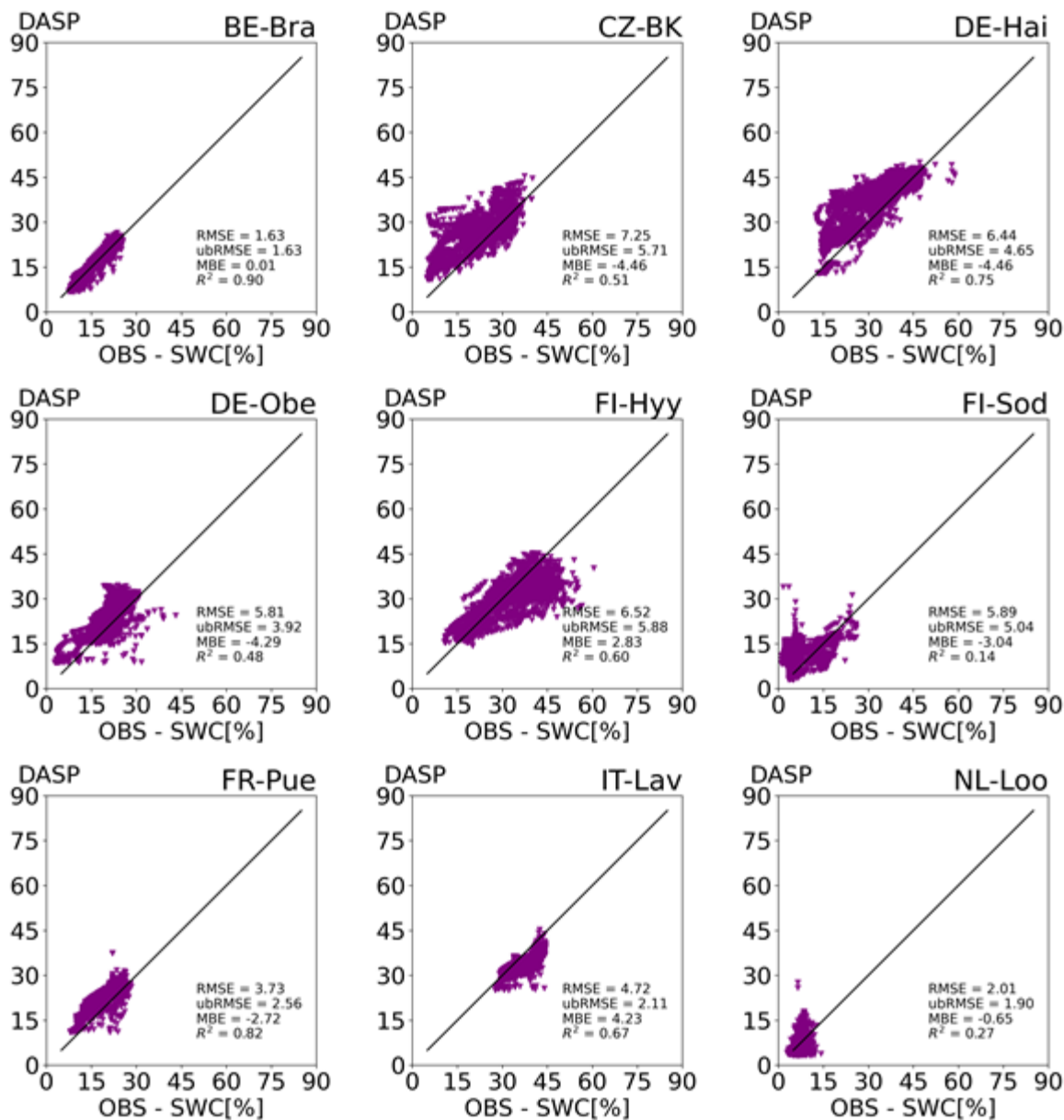



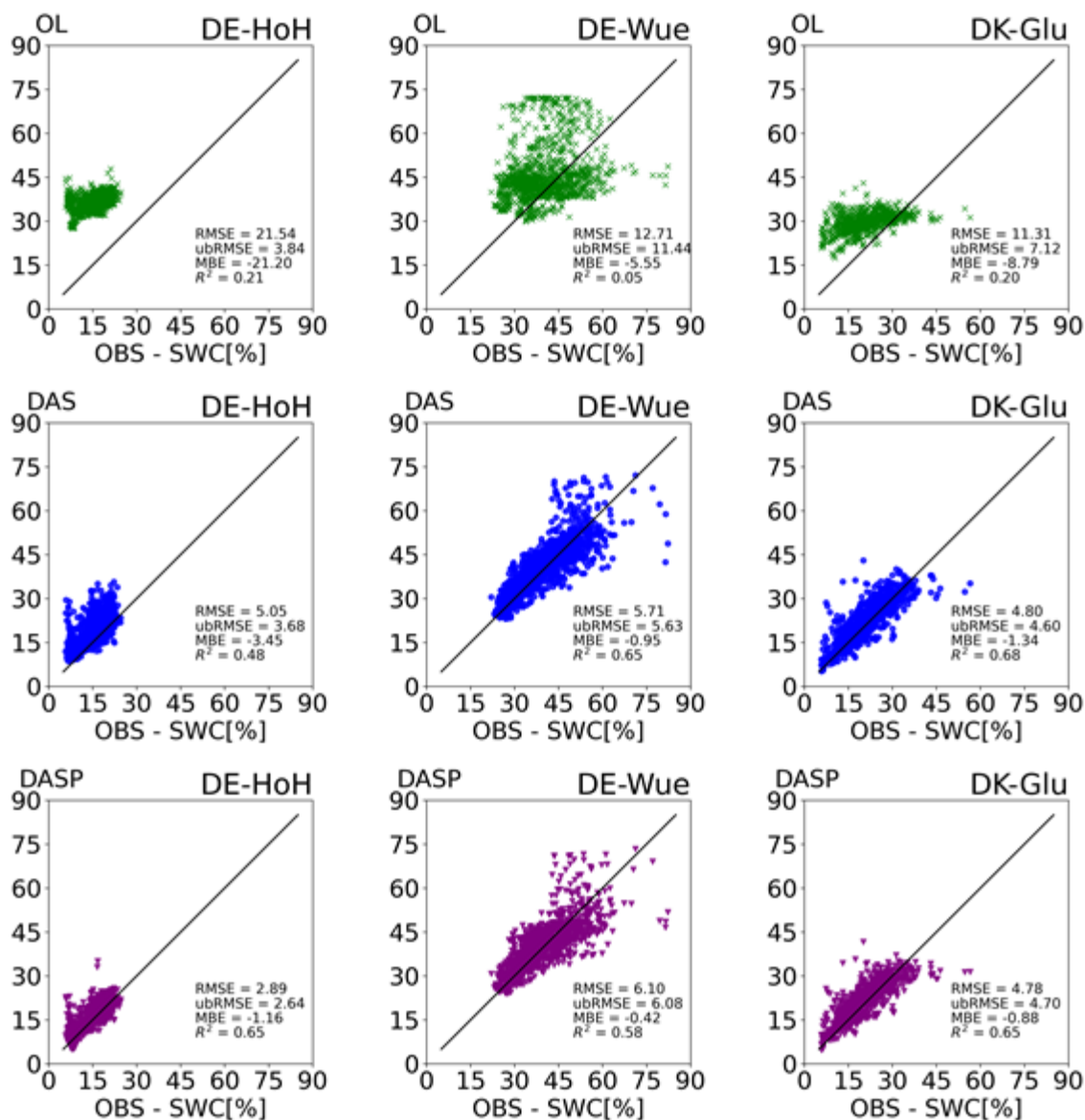
Figure 4: Scatter plots of observed soil water content at nine study sites versus DASP simulation results at 20 cm depth. The points represent daily averages for the days on which observation data are available.

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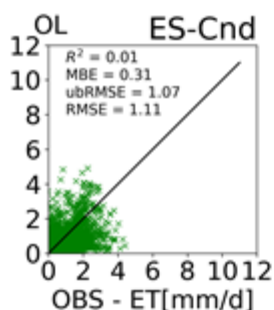
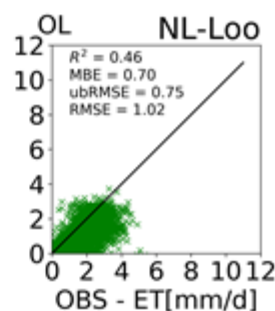
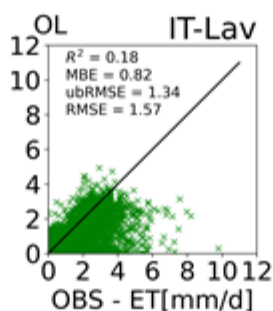
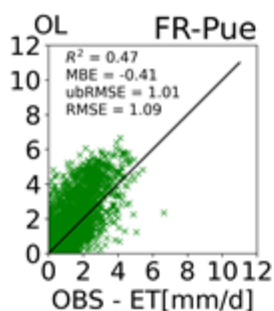
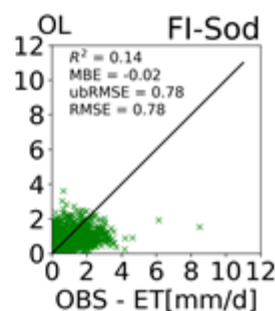
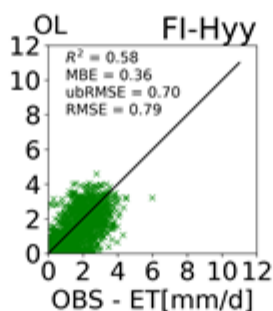
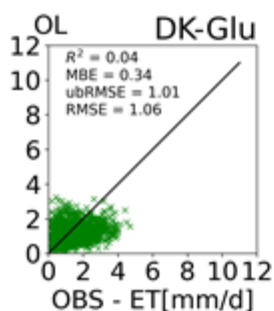
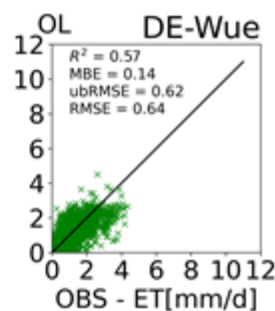
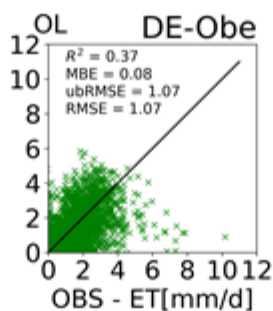
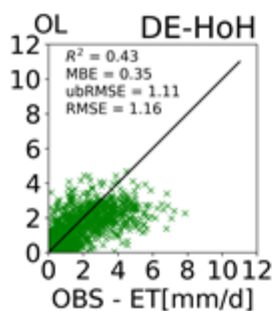
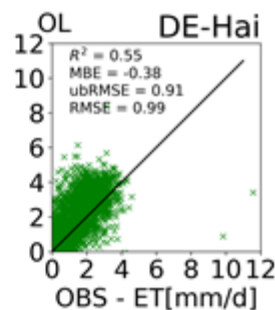
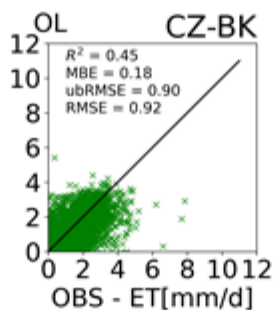
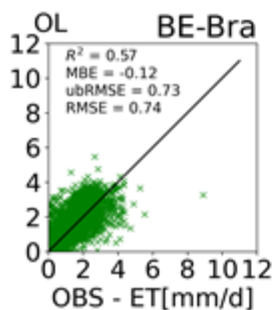
Figure 5: Scatter plots of observed soil water content at three CRNS study sites (DE-HoH left column, DE-Wue middle column, DK-Glu right column) versus simulation results (OL results in the top row, DAS results in the middle row, and DASP results in the bottom row). The points represent daily averages for the days on which observation data are available.

555 **Figure 6: Scatter plots of observed evapotranspiration at thirteen study sites versus OL simulation results. The points represent daily averages for the days on which observation data are available.**

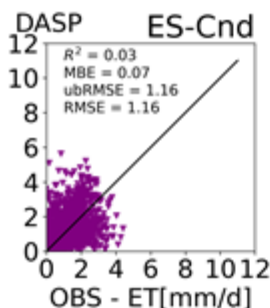
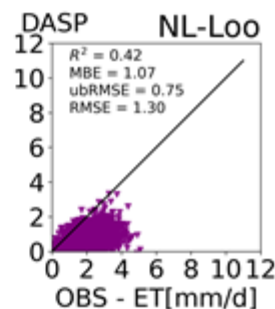
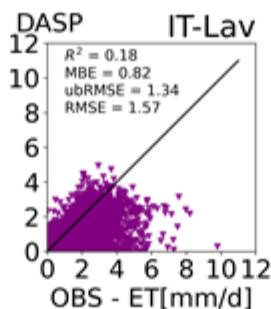
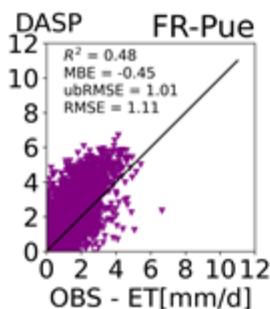
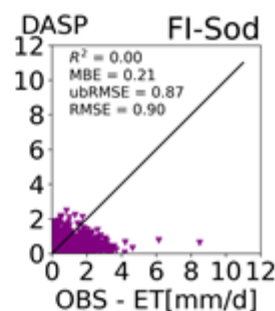
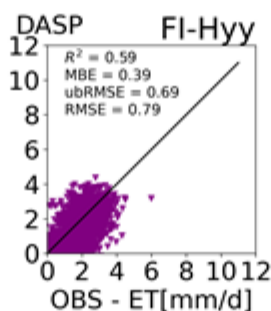
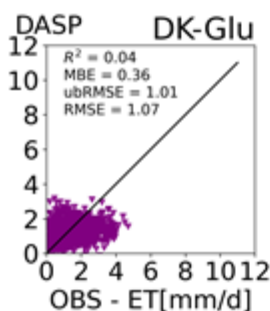
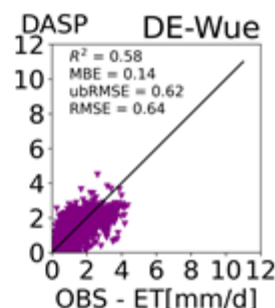
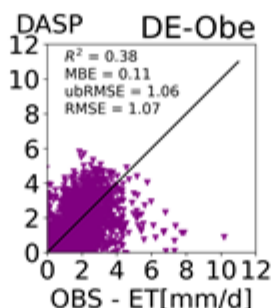
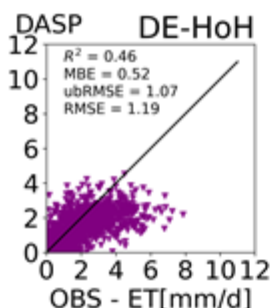
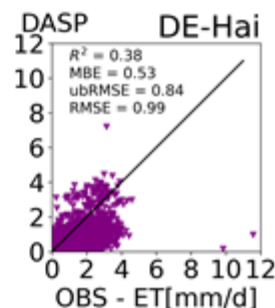
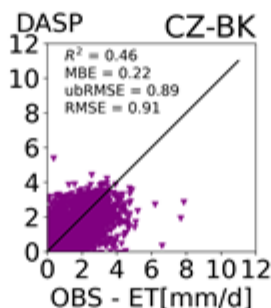
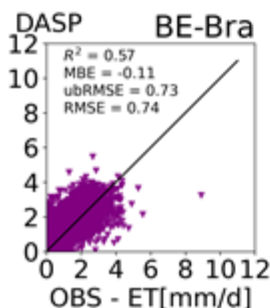



Figure 7: Scatter plots of observed evapotranspiration at thirteen study sites versus DASP simulation results. The points
560 **represent daily averages for the days on which observation data are available.**

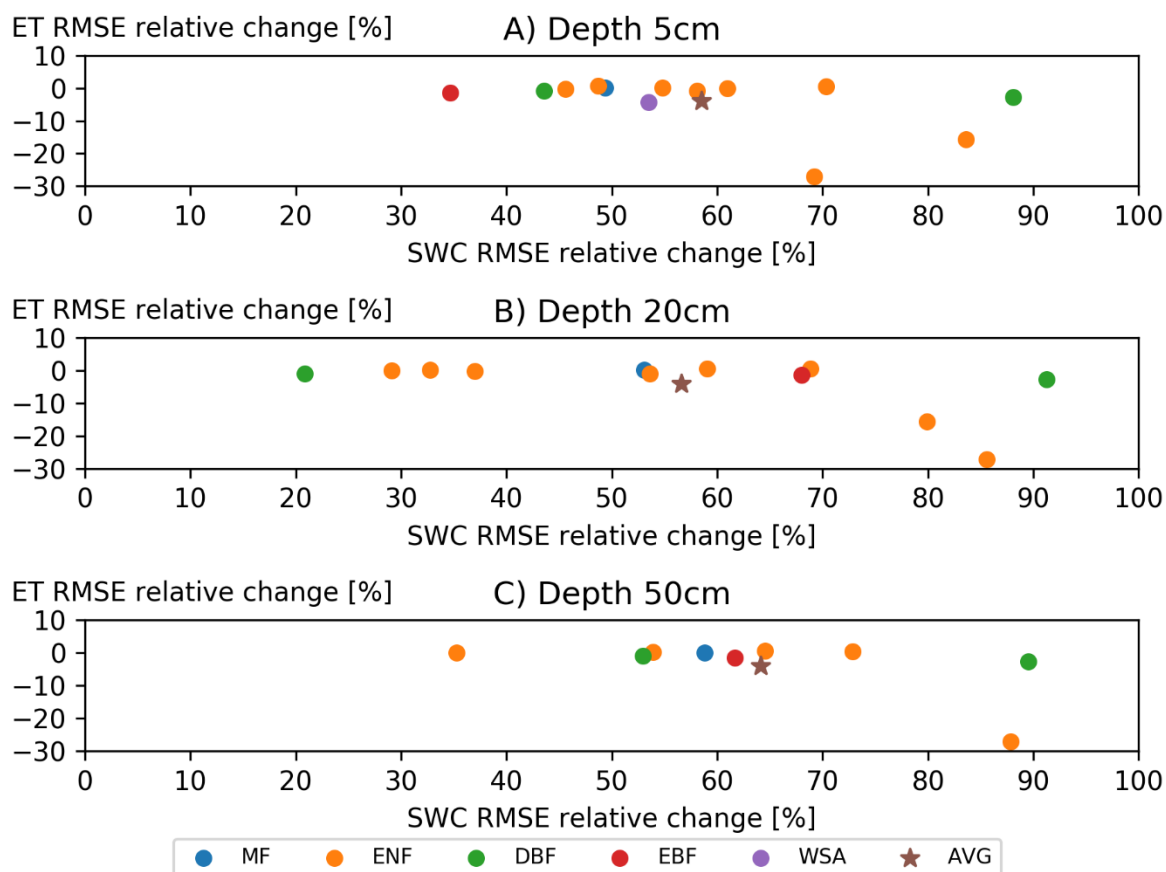



Figure 8: Comparing the SWC and ET characterization for the OL and DASP simulations. Each point represents the overall
average RMSE change for one site. The color of the points indicates the classification code for the different forest types (MF:
mixed forest, ENF: evergreen needle leaf forest, DBF: deciduous broad leaf forest, EBF: evergreen broad leaf forest, AVG:
565 **average over all forest types).**

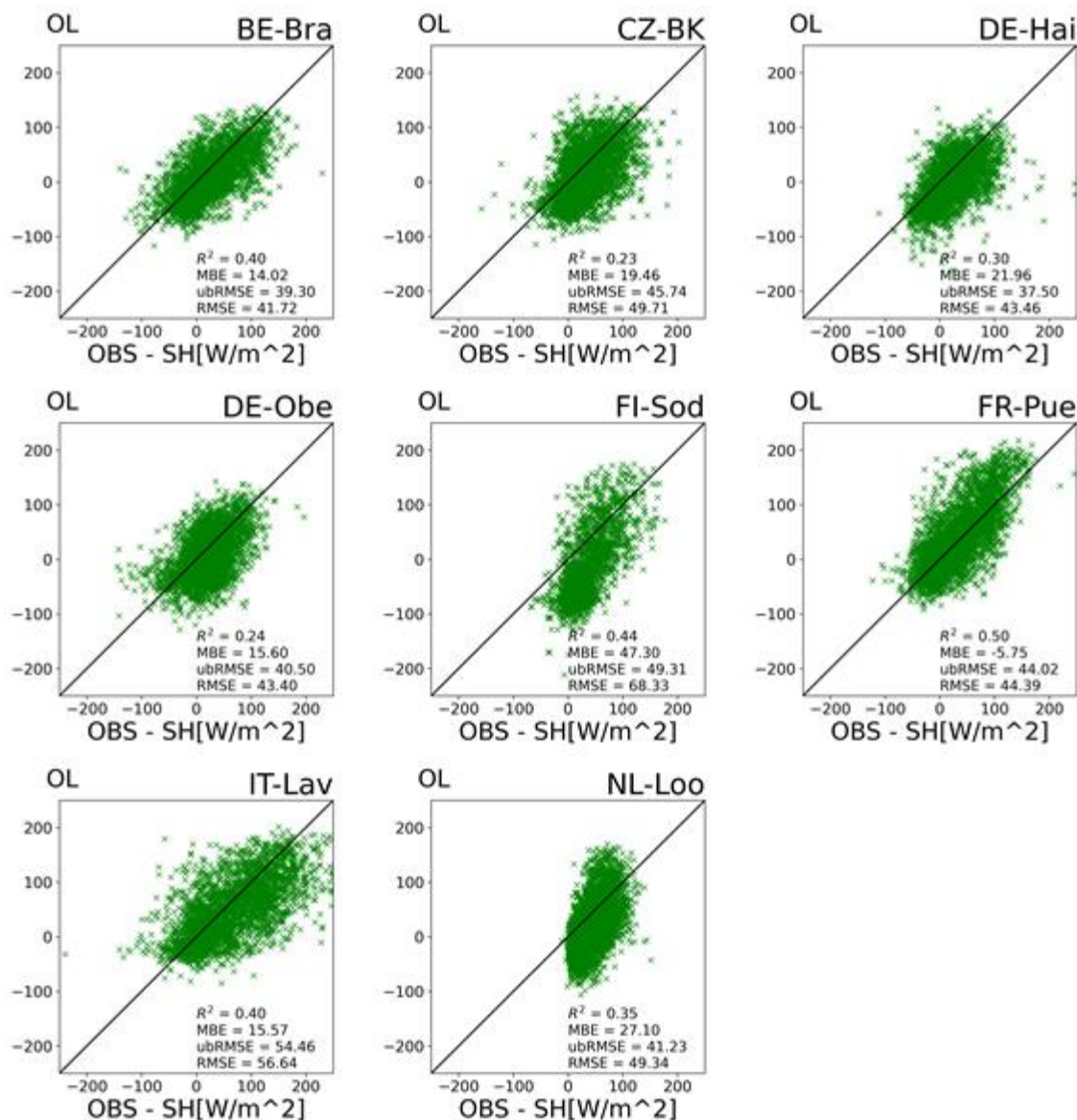



Figure 9: Scatter plots of observed sensible heat flux at eight study sites versus OL simulation results. The points represent daily averages for the days on which observation data are available.

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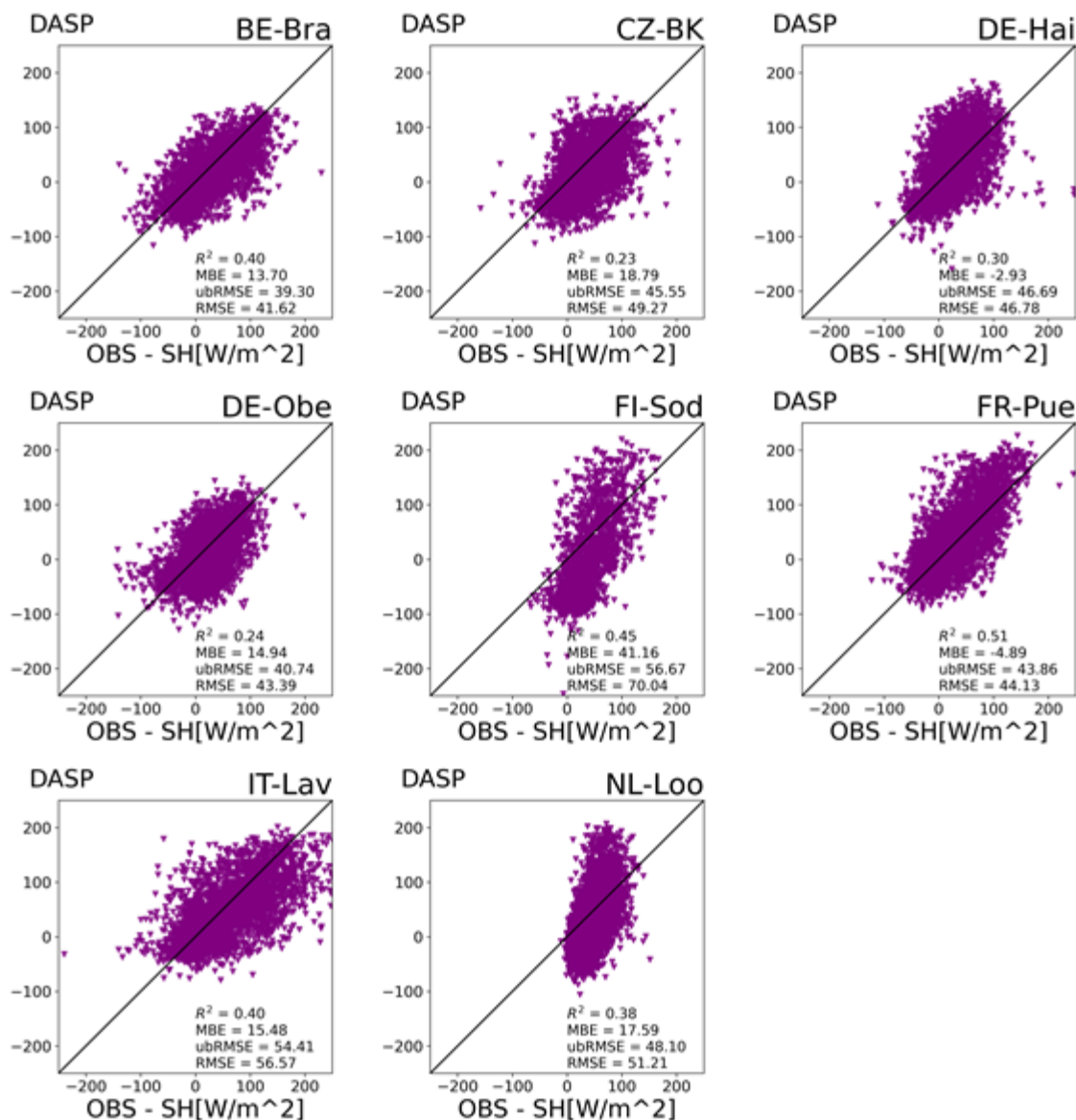
Figure 10: Scatter plots of observed sensible heat flux at eight study sites versus DASP simulation results. The points represent daily averages for the days on which observation data are available.

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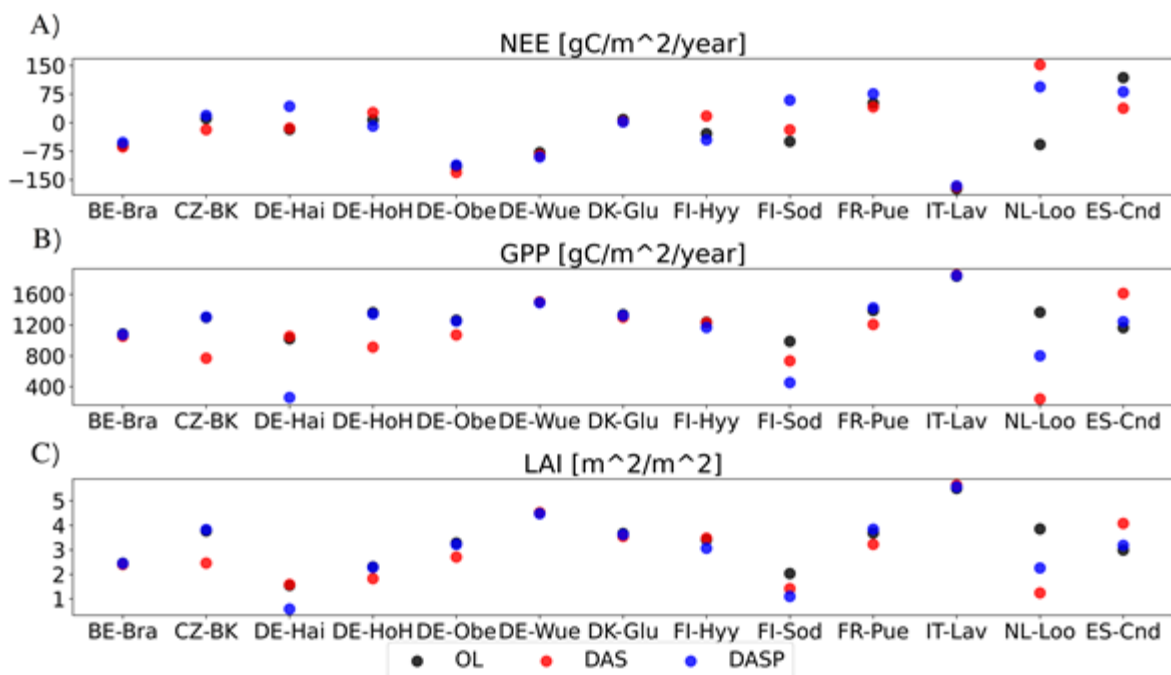
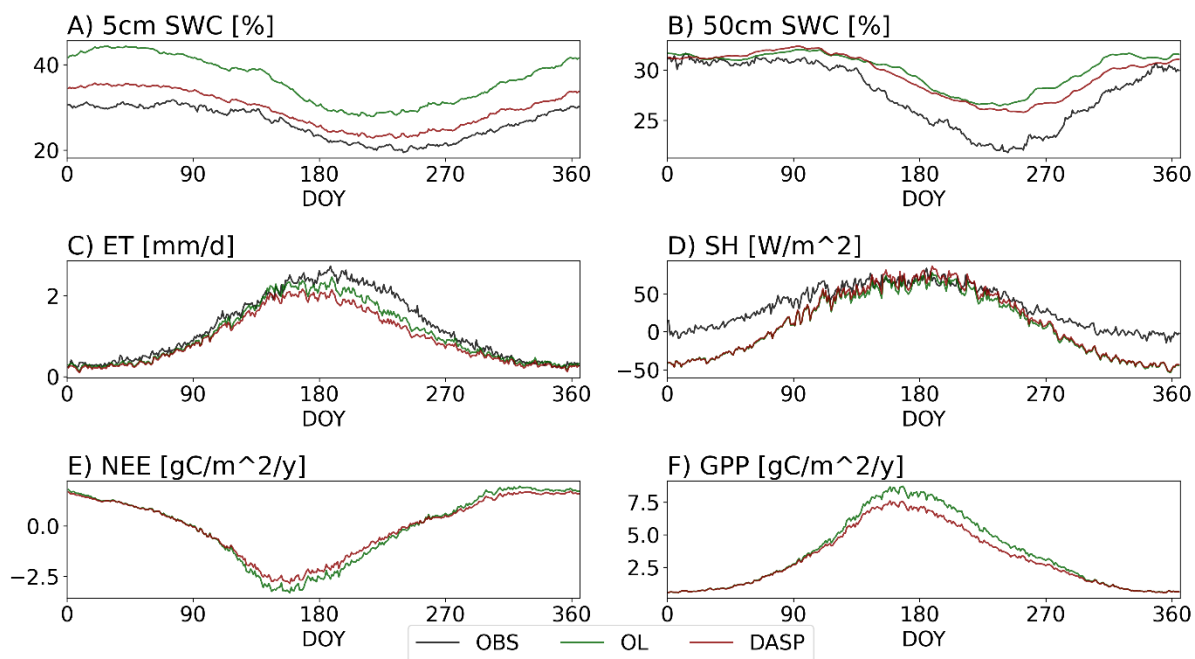


Figure 11: Open loop (OL) and assimilation scenario (DAS and DASP) yearly averages of A) net ecosystem exchange (NEE), B) gross primary production (GPP), and C) leaf area index (LAI) for all selected sites.

580   **Figure 12: Seasonality of observed (OBS) and simulated (OL and DASP) states and fluxes based on daily averages from all years (2009 to 2018) and all sites: A) soil water content (SWC) at 5 cm depth, B) SWC at 50 cm depth, C) evapotranspiration (ET), D) sensible heat flux (SH), E) net ecosystem exchange (NEE), and F) gross primary production (GPP).**

Appendix.

A. Additional figures

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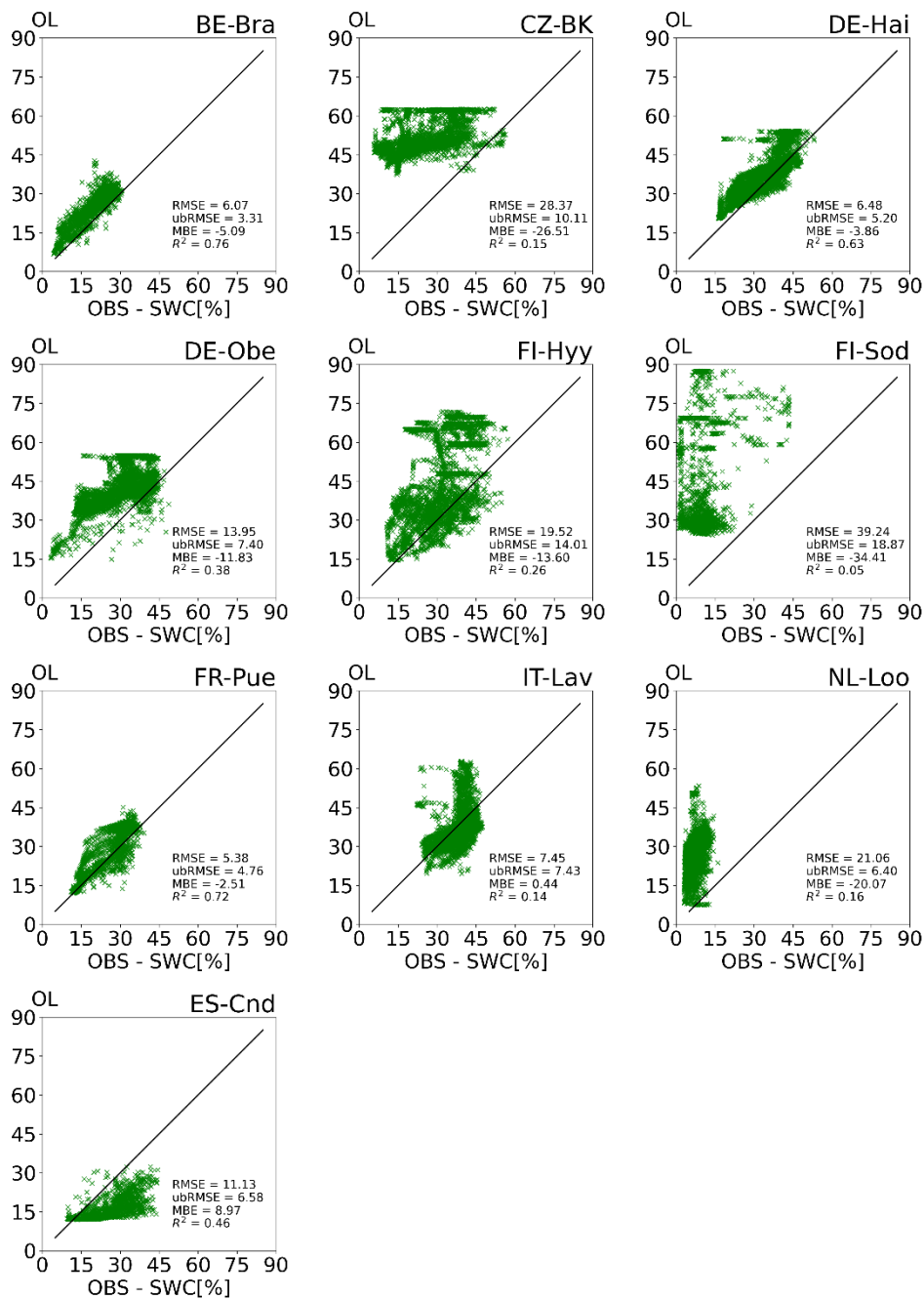
Figure A1 : Scatter plots of observed soil water content at ten study sites versus OL simulation results at 5 cm depth. The points represent daily averages for the days on which observation data are available.
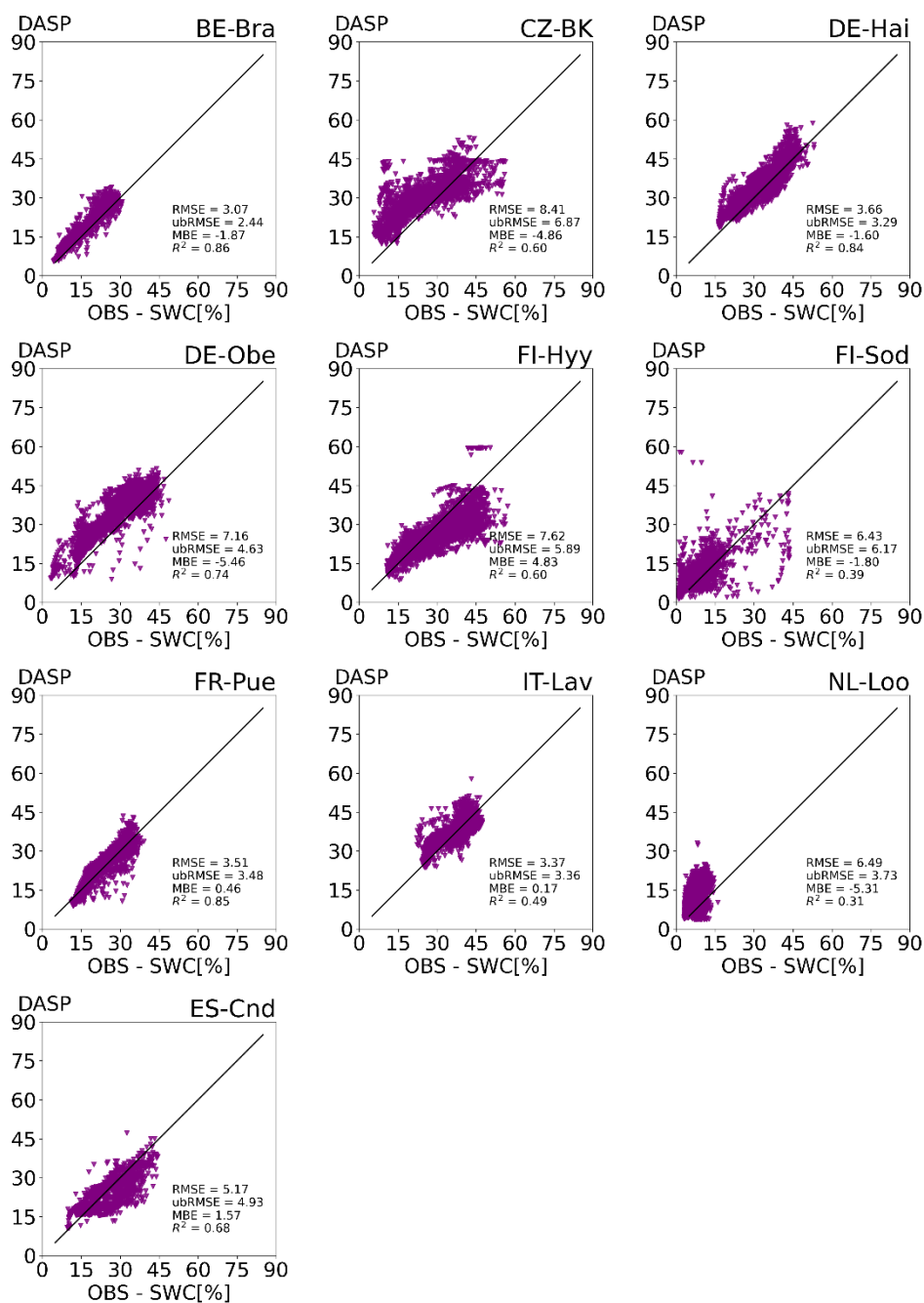
Figure A2 Scatter plots of observed soil water content at ten study sites versus DASP simulation results at 5 cm depth. The points

590   represent daily averages for the days on which observation data are available.
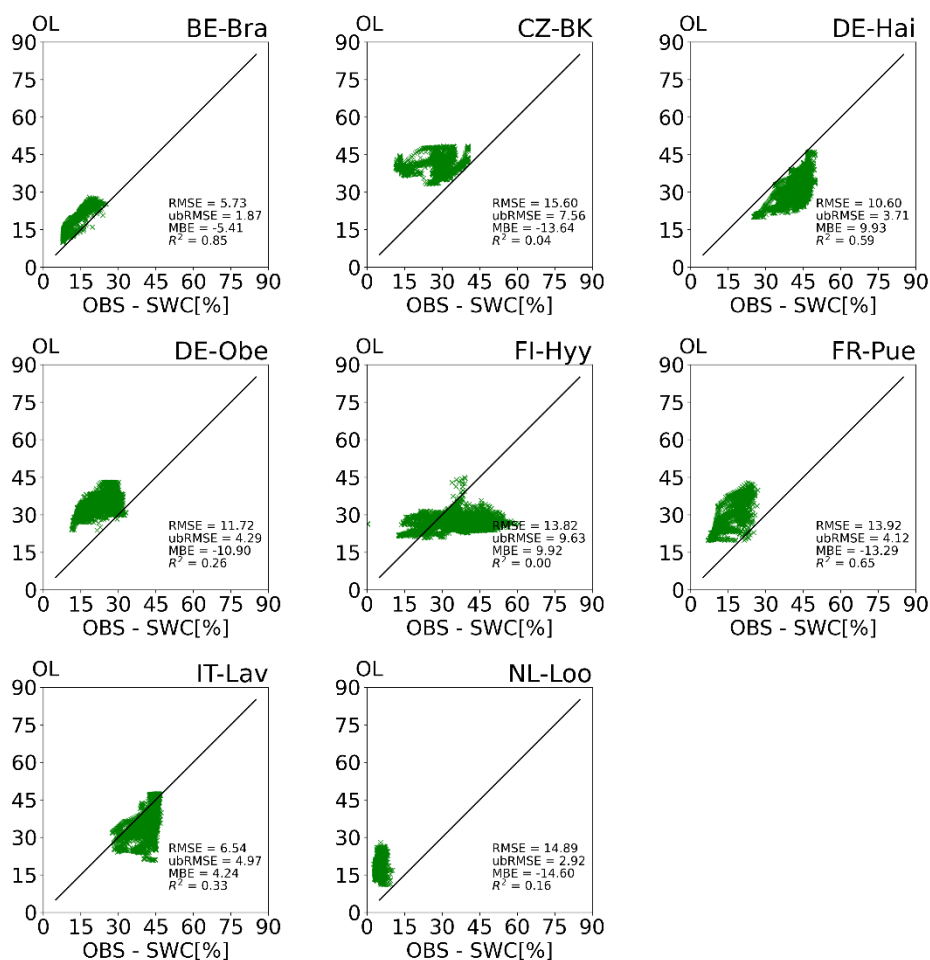
Figure A3: Scatter plots of observed soil water content at eight study sites versus OL simulation results at 50 cm depth. The points

represent daily averages for the days on which observation data are available.

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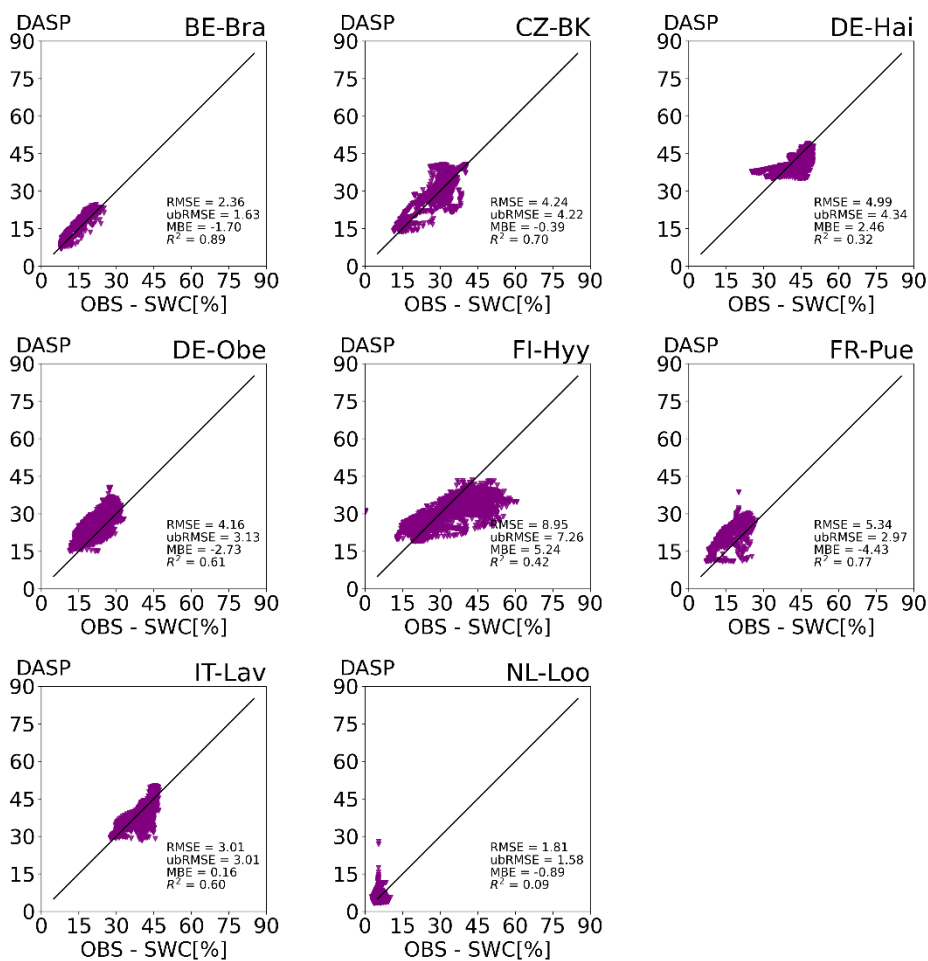
Figure A4: Scatter plots of observed soil water content at eight study sites versus DASP simulation results at 50 cm depth. The points represent daily averages for the days on which observation data are available.

Code availability.

600 The code used in this study is available at https://github.com/HPSCTerrSys/TSMP .

Data availability.

Data for the European FLUXNET sites is available at http://www.europe-fluxdata.eu/. Some additional data used in this study is from the eLTER data portal (https://data.lter-europe.net/) and ICOS data portal (https://www.icos-cp.eu/). The CRNS data is published in "Dataset of COSMOS-Europe: A European network of Cosmic-Ray Neutron Soil Moisture Sensors" available at

605 https://doi.org/10.34731/x9s3-kr48 (Bogena and Ney, 2021).

Competing interests. The authors declare that they have no conflict of interest.

Author contribution.

L.S. pre-processed the data, adjusted the code, performed the simulations, and prepared the manuscript. M.A. and S.A. provided data and contributed to the manuscript. H.B., H.J.H.F., and H.V. supervised the research, co-designed the experiments, and contributed to the manuscript.

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