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Enhancing Hectare-Scale Groundwater Recharge Estimation by Integrating Data From Cosmic-Ray Neutron Sensing Into Soil Hydrological Modeling

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Key Points:

- Calibrating a soil hydraulic model using soil moisture from cosmic-ray neutron sensing (CRNS) allows to simulate hectare-scale groundwater recharge
- Combining CRNS and point-scale sensor profiles increases representativeness of simulated root zone soil moisture and groundwater recharge
- Groundwater recharge estimates from a multi-model ensemble are more consistent than independent estimates using soil water tension data

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Abstract Vadose zone models, calibrated with state variables, may offer a robust approach for deriving groundwater recharge. Cosmic-ray neutron sensing (CRNS) provides soil moisture over a large support volume (horizontal extent of hectares) and offers the opportunity to estimate water fluxes at this scale. However, the horizontal and vertical sensitivity of the method results in an inherently weighted water content, which poses a challenge for its application in soil hydrologic modeling. We systematically assess calibrating a soil hydraulic model in HYDRUS 1D at a cropped field site. Calibration was performed using different field-scale soil moisture time series and the ability of the model to represent root zone soil moisture and derive groundwater recharge was assessed. As our benchmark, we used a distributed point sensor network from within the footprint of the CRNS. Models calibrated on CRNS data or combinations of CRNS with deeper point measurements resulted in cumulative groundwater recharge comparable to the benchmark. While models based exclusively on CRNS data do not represent the root zone soil moisture dynamics adequately, combining CRNS with profile soil moisture overcomes this limitation. Models calibrated on CRNS data also perform well in timing the downward flux compared to an independent estimate based on soil water tension measurements. However, the latter provides quantitative groundwater recharge estimates spanning a wide range of values, including unrealistic highs exceeding local annual precipitation. Conversely, modeled groundwater recharge based on the distributed sensor network or on CRNS resulted in estimates ranging between 30% and 40% of annual precipitation.

Plain Language Summary This study explored how well we can estimate groundwater recharge by modeling how much water moves through the soil after rainfall. To improve the model we used cosmic-ray neutron sensing (CRNS), which measures soil moisture across large areas, and combined it with a soil hydrologic model (HYDRUS 1D) to estimate water movement at a cropped field site. CRNS provides good information on shallow soil moisture, but struggles to capture moisture deeper in the soil. To overcome this, we combined CRNS data with moisture readings from deeper soil sensors. This improved the model's accuracy in predicting water movement through the root zone and into the groundwater. Our findings showed that using CRNS data alone didn't represent deeper soil moisture well enough, but combining it with deeper sensor data produced reliable estimates of groundwater recharge ranging from 30% to 40% of annual rainfall. In contrast, using soil water tension measurements alone resulted in a much wider range of estimates, including some that were unrealistically high. In summary, combining CRNS with deeper soil moisture data improves the accuracy of models used to estimate groundwater recharge, making it a useful approach for understanding water movement in agricultural fields.

1. Introduction

Groundwater recharge is a crucial component within the hydrologic cycle and knowledge about its quantities are of wide spread interest and importance. However, a direct measurement of recharge is difficult. Many methods for its estimation exist, based on either surface water, unsaturated zone or groundwater measurements (e.g., assessment of base flow in discharge, lysimeters, tracers or groundwater table fluctuation). The methods differ in the spatio-temporal scale on which they are able to provide recharge estimates and the choice of an appropriate method depends on the site and target of study (Scanlon et al., 2002). Some of the methods provide estimates for water actually being added to the groundwater storage, others mainly determine deep percolation in the vadose zone, sometimes defined as potential groundwater recharge (Schübl et al., 2023). In this context, different naming conventions exist (Healy, 2010) and in this study we define groundwater recharge as the downward water flux in the vadose zone below the influence of evapotranspiration, that will form actual recharge once reaching the groundwater table.

Variably saturated flow models are one option to assess the water fluxes in the vadose zone and to derive groundwater recharge, often constrained by measured data (Scanlon et al., 2002; Vereecken et al., 2008). They provide time series of groundwater recharge estimates, useful as an upper-boundary condition for groundwater models. A common approach is to calibrate the soil hydraulic model parameters on state variables like soil moisture to then reliably estimate groundwater recharge (Andreasen et al., 2013; T. Wang et al., 2016). Usually, a 1D soil water flux model is adopted to represent the main hydrological processes involved and the scale of the measured data (e.g., soil water content, tension, drainage, evapotranspiration) is directly related to flux estimates at the respective scale (Graham et al., 2018; Jhorar et al., 2004; Lai & Ren, 2016). The soil hydraulic model parameters derived by such inverse modeling are then considered to be "effective," overcoming the difficulties of upscaling soil hydraulic model parameters derived from small soil volumes in the laboratory and are assumed to better represent the average hydrological behavior at the scale of interest (Ritter et al., 2003; Scharnagl et al., 2011; Weber et al., 2024; Wöhling et al., 2008).

For the field or hectare scale, cosmic-ray neutron sensing (CRNS) is a non-invasive technique to obtain soil moisture with at radial footprint of approximately 150 m around the sensor and down to 70 cm depth for completely dry soils. It overcomes limitations of single point-scale sensors that are affected by small-scale heterogeneity. Point-scale sensors only provide a representative field-scale average soil moisture when combined in intensively equipped networks (Rosenbaum et al., 2012). For agricultural sites and especially in cropped fields however, the necessary invasive installation and operation often conflict with regular management practices.

Numerous studies confirm the good performance of CRNS in comparison to point sensor networks especially when weighting the sensor network soil moisture according to the higher CRNS sensitivity close to the sensor and for upper soil layers (Franz, Zreda, Ferre, et al., 2012; Lv et al., 2014). Especially the integration depth, showing an exponential weighting, is dependent on soil water content and for most soils and conditions limited to approximately 30 cm (Franz, Zreda, Rosolem, & Ferre, 2012; Köhli et al., 2015; Schrön et al., 2017; Zreda et al., 2008). In agricultural context, the full root zone soil moisture beyond the CRNS sensing depth is of interest (water fluxes, crop irrigation water requirements), and CRNS therefore has been found most suitable for dry regions with accordingly larger integration depths (Ragab et al., 2017; E. Wang et al., 2018). In other studies, CRNS is assumed to be representative for a fixed but shallow integration depth (e.g., Schreiner-McGraw et al., 2016). Others try to increase the depth representativeness by using an exponential filter (Franz et al., 2020; Peterson et al., 2016) or combine it with few deeper point sensor measurements (Foolad et al., 2017) and temporal stability concepts (Nguyen et al., 2019). Related to the inherent weighting of the CRNS-based soil moisture, Baroni et al. (2018) showed the vertical distribution of soil moisture to be an important source of uncertainty when compared to the simple mean soil moisture of a sensor network. They proposed and tested with good results a "profile shape correction" procedure (Scheiffele et al., 2020), based on a few additional point-scale profile measurements applied to CRNS soil moisture to "unweight" the CRNS signal.

When considering soil hydrological applications, it is difficult to directly compare the integrating average from CRNS to mostly depth specific simulated soil moisture from physically based numerical models. Rivera Villarreyes et al. (2014) overcome this issue by calibrating on water storage, but also assuming CRNS to be representative for a fixed depth. The COSMIC operator (Shuttleworth et al., 2013), developed for data assimilation purposes (Rosolem et al., 2014), accounts for the vertical weighting in the CRNS signal (neutron counts). It has been successfully applied in large-scale land surface models or used for their calibration (Baatz et al., 2017; Fatima et al., 2023; Han et al., 2015; Patil et al., 2021; Schrön et al., 2017). Corresponding to the sensitivity of CRNS, the COSMIC operator represents the topmost soil layers especially well. Since then the COSMIC operator has been implemented into HYDRUS 1D (Brunetti et al., 2019), demonstrating the applicability of CRNS data to derive effective soil hydraulic model parameters for the hectare-scale. A first study by Barbosa et al. (2021) used this to derive groundwater recharge. Both studies show the decreasing representativeness of the simulated to observed soil moisture with increasing depth.

Within this study we systematically assess the effect of several options to integrate the CRNS data in an inverse modeling framework to calibrate the soil hydraulic model (in HYDRUS 1D) and evaluate the resulting simulated soil moisture and hectare-scale groundwater recharge. A distributed sensor network serves as a benchmark, providing high information content in space and time regarding soil moisture and resulting in a highly informed, well-calibrated model. Two different CRNS products will be used for calibration: neutron counts together with the COSMIC operator and the CRNS-derived and thus weighted soil moisture. Additionally, we calibrate the model using two ways of integrating CRNS information with deeper point measurements: a profile corrected CRNS soil moisture and a combination of CRNS and depth specific soil moisture as two independent objectives. To confirm the validity of modeled groundwater recharge rates we compare them to soil water tension-based groundwater recharge as independent estimate, keeping in mind the different spatial scales the methods represent.

We aim to answer the following research questions:

- How well are the soil hydrologic models, calibrated on the different field-scale soil moisture products, able to represent root zone soil moisture?
- How accurately can groundwater recharge be derived using CRNS-based model calibrations, compared to the benchmark estimate using a sensor network and compared to independent tension-based groundwater recharge?
- How large are the uncertainties in the quantitative groundwater recharge estimates from models and soil water tension, considering uncertainties in soil hydraulic model parameters?

The results of this study will offer detailed insights into the use of CRNS data for calibrating physically based soil hydrological models, enabling accurate estimation of field-scale groundwater recharge as well as providing the basis for the study of other fluxes (e.g., evapotranspiration and run off).

2. Materials and Methods

2.1. Field Site and Instrumentation

Data for this study were collected from the agricultural field site Katharinentaler Hof in Southern Germany (48.9285°N, 8.7028°E, elevation 319 m asl) from January 2013 to March 2014. The parent material for the soil formation is loess with a thickness of several meters with the top soil classified as silt loam (USDA soil texture classification). Soil sampling at 16 locations in five regular depth intervals down to 150 cm show a variability in texture with 1%–6% sand, 70%–90% silt and 8%–28% clay. The soil management includes regular plowing or disking, affecting the soil properties of the first 30 cm (Imukova et al. (2016) and Weber et al. (2022)). The groundwater table is about 25 m below the surface, but locally saturated conditions can occur in depths shallower than that. Mean annual temperature is 9.5°C and mean annual precipitation amounts to 780 mm (Imukova et al., 2016; Ingwersen et al., 2011). Weather data were recorded onsite (data available from Weber et al., 2021, 2022). For the period from April to July 2013 a CRNS detector (^{3}He based gas counter, type CRS 1000 from Hydroinnova Ltd, USA) and a distributed soil moisture sensor network (nine-level SM1 capacitance probes from Adcon telemetry, Austria, accuracy ± 2%, termed "sensor network") were run in parallel on the field. At the 15 functioning locations of the sensor network, the water content was measured in 15 min intervals (aggregated to hourly values) at every 10 cm down to 90 cm depth (Imukova et al., 2016). During the measurement period, four campaigns were conducted to collect soil samples for gravimetric determination of soil moisture (16 locations, 9 depths according to the sensor network measurement depths). Bulk density was determined once for individual samples. Texture data was determined on composite samples of 30 cm increments down to 150 cm (Imukova et al., 2016). The soil moisture data were used to assure the fidelity of the capacitance probes as well as to calibrate the CRNS (details see Baroni et al. (2018); Imukova et al. (2016)). The quasi-static additional hydrogen pools (*AHP*) within organic matter and the crystal lattice of the soil minerals, which are required for accurate determination of CRNS soil moisture, were measured from the soil samples by the loss-on-ignition method. Close to the center of the field and the CRNS, four matric potential sensors (257-L, Campbell Scientific Ink., UK) were installed at 130 and 150 cm depth as pairs in a horizontal distance of 50 cm (half hourly data available from Weber et al. (2021, 2022)). Undisturbed soil cores from 140 cm depth were taken to derive soil hydraulic model parameters (Imukova et al., 2016) in an evaporation experiment in the laboratory using a HYPROP system (UMS GmbH, Germany). In 2013, the field was cultivated with winter wheat (*Triticum aestivum L.*) and crop height measurements were acquired on a weekly basis. The in-situ sensors of the sensor network had to be removed shortly before the crop harvest at 4 August. Grubbing and sowing of mustard cover crop on 2 September was followed by plowing on 11 December and bare field conditions for the remaining observation period until end of March 2014.

2.2. Field-Scale Soil Moisture Products

2.2.1. Sensor Network (θ_{SN})

The sensor network composed of capacitive soil moisture sensors provides a point-scale value of volumetric soil moisture for 15 locations distributed within the field and for nine depths each (10–90 cm), representing high horizontal, vertical and temporal resolution (hourly data). The depth specific average of all locations represents the field mean soil moisture profile θ_{SN}.

2.2.2. Neutron Counts From CRNS (NC)

CRNS provides information of field average soil water content by detecting the ambient neutron count rate above ground that is inversely related to soil moisture. The raw neutron count rate measured by the CRNS detector was corrected using standard correction approaches for changes in air pressure, varying incoming neutron flux and air humidity (Rosolem et al., 2013; Zreda et al., 2012), yielding the corrected count rate NC. Hourly neutron counts were subjected to a 12-hr moving average to reduce the statistical noise in the count rate (Zreda et al., 2012).

2.2.3. Weighted Soil Moisture From CRNS (θ_{CRNS})

Converting neutron counts NC to CRNS-derived soil moisture theoretically requires only a one-time calibration of conventionally measuring the water content within the CRNS support volume. This areal average value allows determining the single calibration parameter within the widely used equation from Desilets et al. (2010) (for a more concise mathematical notation see Köhli et al. (2021)). For this study, the calibration parameter was derived using data from four invasive soil moisture sampling campaigns that covered dry, wet and intermediate conditions as recommended by Heidbüchel et al. (2016) and Iwema et al. (2015). The soil moisture from the manual sampling campaigns was weighted according to Schrön et al. (2017) to account for the vertical and horizontal contributions to the CRNS signal. Thus, accounting for the additional hydrogen pools (AHP) and the spatial weighting when calibrating CRNS, the CRNS-derived soil moisture θ_{CRNS} yields a value of horizontally and vertically weighted soil moisture in its support volume (for details on the CRNS calibration at the field site see Baroni et al. (2018) and Scheiffele et al. (2020)).

When comparing θ_{CRNS} to an simple average from the sensor network $\overline{\theta_{SN}}$, the inherent weighting in θ_{CRNS} leads to deviations between the two time series, especially for situations with pronounced gradients in the soil moisture profile (Baroni et al., 2018). To achieve comparability between the two time series, usually the point-scale data are weighted according to their depth and distance to the CRNS according to its spatial sensitivity.

2.2.4. Profile Corrected Soil Moisture From CRNS (θ_{CRNSpc})

For a comparison between θ_{CRNS} and point scale data, previous studies have shown the vertical weighting to be of higher importance than the horizontal weighting for otherwise homogeneous field sites (Baroni et al., 2018; Franz et al., 2013). Baroni et al. (2018) proposed to reduce the vertical sensitivity in the CRNS-derived soil by "unweighting" θ_{CRNS} using information of the soil moisture profile:

$$\theta_{CRNSpc} = f_{pc} \cdot \theta_{CRNS} - AHP \;\; ; \;\; f_{pc} = \overline{\theta_{SN}} / \theta_{SN,vwt} \tag{1}$$

where the correction factor f_{pc} for each time step is based on the ratio of the arithmetic mean soil moisture of a vertical profile ($\overline{\theta_{SN}}$) and its vertically-weighted soil moisture $\theta_{SN,\mathrm{vwt}}$ (weighting according to Schrön et al. (2017)). This yields the profile corrected CRNS soil moisture θ_{CRNSpc}. In this study, we calculated f_{pc} based on the depth specific average of all 15 sensor network locations as representative soil moisture profile θ_{SN}. Scheiffele et al. (2020) showed this "unweighting," when based on a few measured soil moisture profiles, to achieve a good comparability to the average soil moisture from a sensor network.

2.3. Model Structure and Calibration

2.3.1. HYDRUS 1D Setup

The soil hydrological processes were simulated using the variably saturated flow model in HYDRUS 1D (Šimůnek et al., 2008). It is based on the Richards equation including root water uptake, and in this study we parametrized the soil hydraulic model of Van-Genuchten-Mualem (van Genuchten, 1980). The soil hydraulic model parameters (residual water content θ_r (cm^3 cm^{-3}), saturated water content θ_s (cm^3 cm^{-3}), the inverse to the air entry pressure α (cm^{-1}), the pore size distribution index n (−), saturated hydraulic conductivity Ks (cm d^{-1}), and a pore-connectivity parameter and l (−)) describe the shape of the matric-potential-dependent soil water retention $\theta(h)$ and unsaturated hydraulic conductivity $K(h)$ functions (van Genuchten, 1980).

The modeled timespan comprised a spin-up period (January to March 2013), the calibration period (April to July 2013) and a period of model application (August 2013 to March 2014) to cover a full year after the model spin-up. The model domain extended from the soil surface down to 150 cm depth with a spatial discretization of 1 cm. We distinguished two soil layers (0–30 cm as plow layer, 31–150 cm according to soil properties and texture (Imukova et al. (2016) and Weber et al. (2022)). The initial conditions (1st January 2013) are set close to field capacity for the entire soil column, that is, a water content of 0.32 cm^3 cm^{-3}. Boundary conditions were set to a free drainage boundary at the bottom and a time variable atmospheric boundary (daily precipitation and temperature) with surface runoff at the top. Potential evapotranspiration was calculated within HYDRUS using the Hargreaves formula (Hargreaves, 1994).

Root water uptake during the spin-up and calibration period was simulated using the Feddes equation (Feddes et al., 1978) with the parameters for wheat, whereas for the mustard cover crop in the model application time the parameters for Alfalfa were applied as proxy. Crop height measurements for winter wheat were available from weekly to biweekly measurements, linearly interpolated to derive daily values. Root growth for wheat was approximated by a linear increase in root depth from 40 cm in January to 80 cm in April (Asseng et al., 1997). Root density shows usually a rapid decrease with depth and even though some roots can grow deeper the 80 cm can be considered the effective rooting depth of the crop (Asseng et al., 1997; Palosuo et al., 2011). The observed agricultural operations during the model application period were parametrized accordingly (Section 2.1). We kept the soil hydraulic model parameters constant, as soil management commonly only causes short-term changes to soil hydraulic properties, with a few wetting-drying cycles being sufficient to restore the original state (M. Zhang et al., 2017). Linear growth is assumed for the mustard cover crop for plant height, cover fraction and root length with values taken from literature (Bodner et al., 2013; Brennan & Smith, 2018; De Baets et al., 2011). The downward water flux over the lower model boundary (bottom flux) represents the simulated groundwater recharge.

2.3.2. COSMIC Operator

The COsmic-ray Soil Moisture Interaction Code (COSMIC; Shuttleworth et al., 2013) is a forward analytical neutron transport approximation, developed for data assimilation (Rosolem et al., 2014) and the model accounts for the decreasing representativeness with depth contained in the CRNS data. The COSMIC operator was implemented into HYDRUS 1D where it computes a neutron count rate from simulated soil moisture. It has shown to be of value for the inverse estimation of soil hydraulic model parameters (Brunetti et al., 2019). Its model parameters are adjusted using site-specific information of field average bulk density (for the field in this study 1.51 g cm^{-3}). The scaling parameter N_{COSMIC} adjusts the absolute count rate simulated with COSMIC to the measured neutron count rate, that is, accounting for CRNS sensitivity. N_{COSMIC} was fixed at 254 counts per hour based on forward simulations of the soil hydraulic model in HYDRUS.

2.3.3. Soil Hydraulic Model Parameters

Initial estimates for the soil hydraulic model parameters in the plow layer were derived based on soil texture (sand, silt, clay fractions) and bulk density data from the soil sampling campaigns (Section 2.1) using the pedotransfer function ROSETTA (Y. Zhang & Schaap, 2017). We derived parameter values based on individual samples and used the average value as initial estimate (Table 1). For the bottom layer parameters were determined from the evaporation experiment in the laboratory using the undisturbed soil cores obtained at a depth of 140 cm (Section

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Table 1
Initial Estimates of Soil Hydraulic Model Parameters and the Parameter Bounds for the Model Calibration

				Parameter bounds	
			Initial estimate	Lower	Upper
Plow layer (0–30 cm)	θ_r	cm^3 cm^{-3}	0.082	fixed	
	θ_s	cm^3 cm^{-3}	0.430	0.30	0.54
	α	cm^{-1}	0.004	0.001	0.100
	n	–	1.5	1.10	2.00
	Ks	cm d^{-1}	19.0	0.1	100
	l	–	0.5	fixed	
Bottom layer (31–150 cm)	θ_r	cm^3 cm^{-3}	0.069	fixed	
	θ_s	cm^3 cm^{-3}	0.432	0.30	0.54
	α	cm^{-1}	0.0064	0.001	0.100
	n	–	1.61	1.10	2.00
	Ks	cm d^{-1}	10.40	0.10	100
	l	–	0.5	fixed	

Note. θ_r: residual water content (cm^3 cm^{-3}), θ_s: saturated water content (cm^3 cm^{-3}), Ks: saturated hydraulic conductivity (cm d^{-1}), α: inverse of the air entry pressure (cm^{-1}), n: pore size distribution index (−), l pore-connectivity parameter (−). θ_r and l were fixed at initial estimates and not calibrated.

2.1, Imukova et al., 2016). The uncalibrated model running with this initial parameter set is termed the" **baseline model**."

For model calibration, parameter bounds for the most sensitive parameters were determined using ROSETTA estimates based on individual soil samples (max. and min. parameter estimate ±2 sd). Some ranges were moderately increased to allow the global optimizer (Section 2.3.4) to find solutions without touching parameter bounds (Table 1). Ranges are comparable to other studies using global optimization to determine soil hydraulic model parameters (e.g., Brunetti et al. (2019) with ranges for silty to loamy soil).

2.3.4. Global Optimizer and Objective Function

HYDRUS 1D allows for internal, inverse soil hydraulic model parameter estimation (i.e., calibration) using the Marquardt-Levenberg algorithm (Levenberg, 1944; Marquardt, 1963), a gradient-based local search method. In a complex parameter space, such gradient-based optimization algorithms are sensitive to the initial parameter estimates and therefore might only find a local minimum. External optimization using global search algorithms can overcome this problem also within HYDRUS (Brunetti et al., 2016; Rivera Villarreyes et al., 2014). Recently, Brunetti et al. (2022) demonstrated a successful global-local search algorithm, coupling a comprehensive learning swarm with the Marquardt-Levenberg algorithm within HYDRUS, but this option is not implemented in the freely available version of the program.

For our study, an external global optimization using a particle swarm optimization (Kennedy & Eberhart, 1995; Kennedy et al., 2001) was applied (as implemented in R-package "ppso," Francke, 2020). The swarm was set up with 70 particles (Piotrowski et al., 2020) and configured for a maximum of 5,000 model evaluations. A convergence criterion was set, but as often observed in environmental models (Mai, 2023) the algorithm was mostly aborted because the maximum number of model evaluations was reached. The Kling-Gupta efficiency (KGE, Gupta et al., 2009; Kling et al., 2012) between simulated and observed soil moisture was the objective function to be maximized as a measure of goodness-of-fit. HYDRUS runs based on parameter sets that did result in non-convergence of the numerical model and those with a mass balance error larger than 1%, were not considered further in the optimization.

While we stayed with the KGE as objective function, we also tracked other performance measures: NSE—Nash-Sutcliffe-Efficiency ($-\infty$ to 1, with 1 being the optimal fit); MAE—Mean absolute error and RMSE—root mean square error (in units of compared variable, 0 being the optimal fit); R^2—coefficient of determination (0–1, with 1

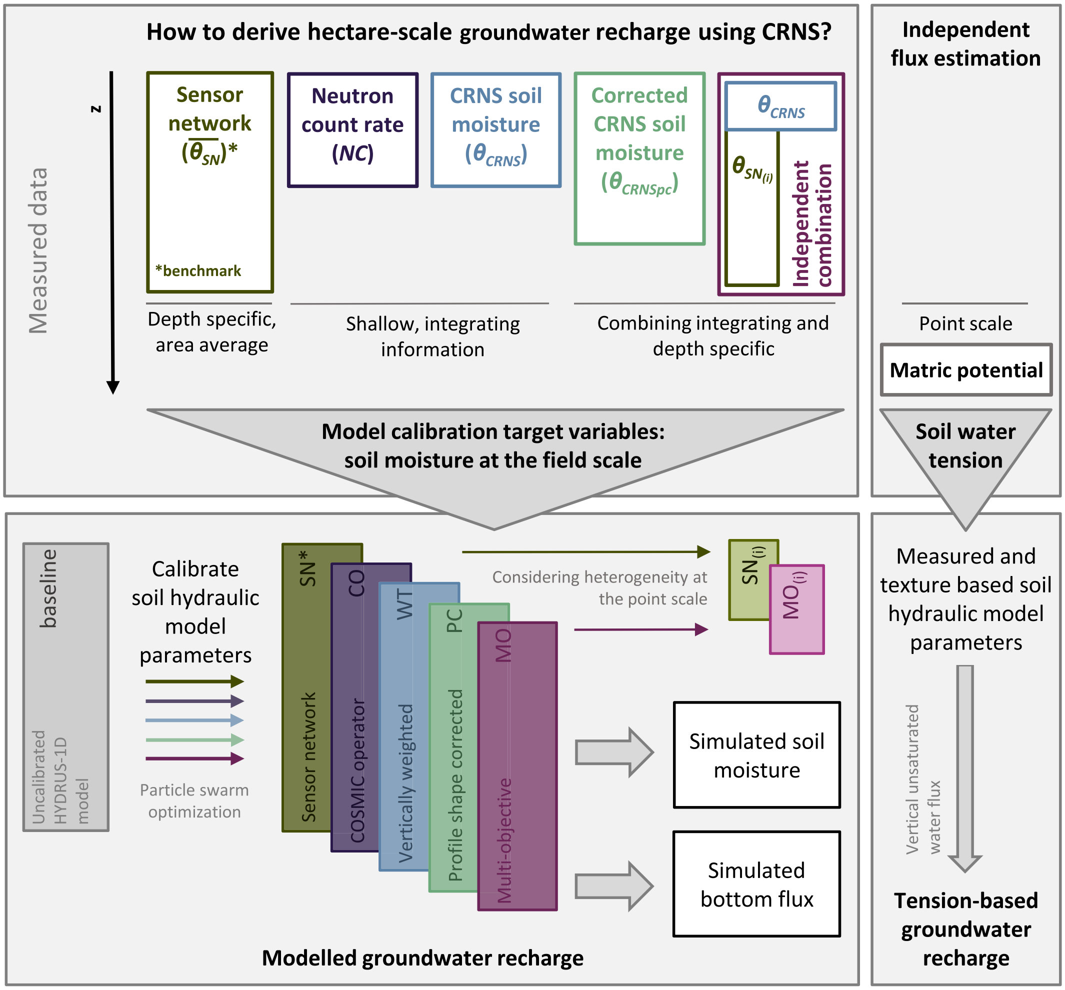

Figure 1. Workflow of the study. Different field-scale soil moisture products are used as target variables for the model calibration, resulting in different models (i.e., sets of soil hydraulic model parameters) and corresponding estimates of hectare-scale groundwater recharge. An independent point-scale estimate of groundwater recharge is derived using soil water tension measurements.

being the optimal fit). For a discussion on choosing one or the other and the effect on the model calibration see for example, Chai and Draxler (2014), Knoben et al. (2019), Mai (2023).

As the measured soil moisture in this agricultural setting was only available during the growing season, we restrained from splitting the 4 months into a calibration and validation data set. The calibration validation concept anyway has been under discussion and Arsenault et al. (2018) and Shen et al. (2022) could show best calibration results when using all available data for large-scale studies.

2.4. Calibration Scheme and Uncertainty in Modeled Groundwater Recharge

Starting from the uncalibrated **baseline** model, the different field-scale soil moisture products (Section 2.2) were used as target variables for the soil hydraulic model calibration. Figure 1 gives an overview of the workflow of the study from target variables to calibrated models and the comparison to an independent groundwater recharge estimate based on the soil water tension measurements (Section 2.5).

The data of the sensor network provide the highest information content in respect to depth and horizontal coverage and thus their depth-specific average θ_{SN} (Section 2.2.1) served as a benchmark measurement. θ_{SN} is directly comparable to the simulated soil moisture from HYDRUS 1D in the respective depths. The model calibrated on θ_{SN} serves as benchmark model (**model SN**).

To calibrate the model on CRNS data, the HYDRUS output has to be modified to represent a similarly aggregated information. This can be achieved by comparing the observed neutron count rate *NC* (Section 2.2.2) to the simulated neutron counts from the COSMIC operator as implemented in HYDRUS 1D (**model CO**). As second calibration option using solely CRNS data, we utilized the CRNS-derived soil moisture θ_{CRNS} (Section 2.2.3) and weighted the HYDRUS simulated soil moisture for each time step according to the vertical sensitivity (weighting following Schrön et al. (2017)) of the CRNS (**model WT**).

We also used a combination CRNS and point-scale data as target variables in two different ways. To derive θ_{CRNSpc} the point-scale soil moisture profile is used to "unweight" the CRNS data (Section 2.2.4) and in the calibration procedure we thus compare it to the average simulated soil moisture over 0–60 cm (**model PC**). As second option, we calibrated the model on more than one target variable, that is, a multi-objective calibration (**model MO**). We tested the combined use of (a) θ_{CRNS}, assumed to be representative of an integration depth of 20 cm, and (b) an average soil moisture profile, derived from three locations of the sensor network randomly selected within a radius of 100 m, as suggested by Scheiffele et al. (2020). Averaging the goodness-of-fit measures (KGE) for both target variables reduces the two objectives to a single-objective problem with the compromise solution located at the pareto-front (Mai, 2023). Table 2 summarizes the calibration approach and the IDs for the differently calibrated soil hydraulic models as well as information on how HYDRUS output is compared to the target variables.

The calibration for the different target variables resulted in varying soil hydraulic model parameter sets (Section 3.1). These models were compared with regard to their ability to overcome the inherent limitation of CRNS in respect to its depth representativeness and in particular, to represent root zone soil moisture also in larger depths (Section 3.2). Furthermore, their respective groundwater recharge estimates were compared to those from the benchmark model SN and to an independently estimated groundwater recharge from soil water tension (Section 3.3). Finally, we estimated the uncertainty in the simulated groundwater recharge (Section 3.4).

Despite the global optimization used for calibrating the soil hydraulic model, the issue of equifinality, as often observed in environmental models (Khatami et al., 2019; Mai, 2023), needs consideration. This phenomenon implies that the optimized parameter set is potentially just one of several equally valid sets that yield the same performance when compared to observations (Beven & Binley, 1992). This could result in substantial differences in the estimated downward flux constituting groundwater recharge (Moore et al., 2010). We thus repeated the optimization for each model (SN, CO, WT, PC, MO) 10 times which, due to the stochastic nature contained in the particle swarm optimization, results in different parameter sets. Assessing the convergence of the goodness-of-fit and of the soil hydraulic model parameters to similar values within these repeated optimizations informs about the robustness of the calibration setup and the identifiability of the parameters by the given data. While these replicates of the optimization provide a range in groundwater recharge estimates, it is not a classical uncertainty analysis, where uncertainties that arise from model assumptions or the uncertainty in the input data are taken into account. Instead, it rather allows to systematically test the robustness of the parameter estimation when utilizing integrating soil moisture products based on CRNS in model calibration (CO, WT, PC, MO) compared to the benchmark case (SN) and evaluate their modeled groundwater recharge and root zone soil moisture representation.

To address the aspect of uncertainty, we assessed the small-scale heterogeneity and resulting variability of the soil properties within the field (see also Table 2), by using soil moisture data from single locations of the sensor network as target variables in the calibration (**model** $\mathbf{SN_{(i)}}$, with i varying from 1 to 10). The soil moisture profiles of the 10 locations closest to the CRNS detector were used (radial distance <100 m), which is the area that dominates the CRNS signal. Analogously, the multi-objective calibration is varied in the same way, combining θ_{CRNS} with soil moisture profile data of the 10 closest locations from the sensor network ($\mathbf{MO_{(i)}}$, with i varying from 1 to 10).

Additionally, we assess the overall uncertainty in modeled groundwater recharge rate by evaluating the range in groundwater recharge from the multi-model ensemble (Groh et al., 2020) consisting of the models calibrated on different field-scale soil moisture products and compare it to the independent groundwater recharge estimate from soil water tension (Section 2.5).

Table 2
Calibration Scheme Using Different Field-Scale Soil Moisture Products as Target Variables for Calibrating the Soil Hydraulic Model, Model IDs and the Way the Simulation Results From HYDRUS 1D Are Modified to be Appropriately Comparable to the Field-Scale Soil Moisture Products

Model ID (soil hydraulic model parameter sets)	Target variable	HYDRUS output used for deriving the objective function value (KGE) in the optimization	Calibration scheme
Baseline	–	–	Uncalibrated
SN	Sensor network mean profile θ_{SN}	Simulated depth specific soil moisture at observation depths of θ_{SN}	Each calibration repeated 10 times to assess the uncertainty from the calibration and resulting equally valid parameter sets in groundwater recharge estimates
CO	Neutron counts *NC*	Simulated neutron count rate, as obtained from simulated soil moisture by the COSMIC operator	
WT	CRNS soil moisture θ_{CRNS} (inherently weighted)	Simulated soil moisture weighted according to CRNS sensitivity	
PC	Profile corrected CRNS soil moisture θ_{CRNSpc}	Average of simulated soil moisture over 0–60 cm depth	
MO	Multi-objective: combining θ_{SN} and θ_{CRNS}	KGE = 0.5 (KGE_1 + KGE_2) KGE_1 = average simulated soil moisture 0–20 cm depth KGE_2 = simulated depth specific soil moisture, at observation depths of θ_{SN}	
$SN_{(i)}$	A single profile of the sensor network $\theta_{SN(i)}$	Simulated depth specific soil moisture at observation depths of $\theta_{SN(i)}$	Assessing variability within the field and uncertainty in groundwater recharge
$MO_{(i)}$	Combining a single sensor network profile $\theta_{SN(i)}$ and θ_{CRNS}	KGE = 0.5 (KGE_1 + KGE_2) KGE_1 = average simulated soil moisture 0–20 cm depth KGE_2 = simulated depth specific soil moisture, at observation depths of $\theta_{SN(i)}$	

Table 3
Soil Hydraulic Model Parameters From the Evaporation Experiment and, Based on Soil Texture Data and Pedotransfer Function (ROSETTA), Parameter Ranges for the Uncertainty Analysis on Tension-Based Groundwater Recharge

				Parameter ranges derived from pedotransfer functions	
		Evaporation experiment based	Texture-based average	Lower	Upper
θ_r	cm^3 cm^{-3}	0.069	Fixed to the measured value 0.069		
θ_s	cm^3 cm^{-3}	0.432	0.41	0.36	0.47
α	cm^{-1}	0.0064	0.013	0.006	0.020
n	–	1.61	1.4	1.20	1.61
Ks	cm d^{-1}	10.40	20	3	39
l	–	0.5	Fixed to 0.5		

2.5. Groundwater Recharge From Soil Water Tension and Associated Uncertainty

It is considered good practice to estimate groundwater recharge applying multiple methods. While the quantitative estimate might differ largely between the methods (Walker et al., 2019), they may still show a consistency and support the validity of the estimate, in our case the modeled groundwater recharge.

We derived an independent groundwater recharge estimate using the data from the matric potential sensors. Their installation depth is approximately equal to the lower model boundary. The half hourly measurements of the matric potential or soil water tension (expressed in pressure head h) below the root zone together with estimates of the soil hydraulic properties can be used to determine the water flux in the unsaturated zone (Healy, 2010; Rolston, 2007):

$$\mathrm{q} = -\mathrm{K}\,(h) \cdot \left(\frac{h_{130} - h_{150}}{\Delta z} + 1 \right) \tag{2}$$

where $K(h)$ is the vertical unsaturated hydraulic conductivity (in cm d^{-1}), h_{130} and h_{150} (in hPa) are the pressure heads at depths of 130 and 150 cm, respectively, and Δz is the vertical distance between the matric potential sensors. The soil hydraulic model parameters used to parameterize $K(h)$ are shown in Table 3. The flux calculations were aggregated to hourly values (q in mm h^{-1}). The downward water flux below the root zone represents a tension-based groundwater recharge estimate and while it provides a comparative flux estimate to the model simulation, they operate on different spatial scales.

The derivation of the soil hydraulic model parameters based on small soil cores in the laboratory contains substantial uncertainty, from fitting the continuous function to the measured data (Peters & Durner, 2008) and regarding their scale representativeness (Weber et al., 2024). While pedotransfer functions are also known to result in unexplained variability in soil hydraulic parameters (Vereecken et al., 2010), the texture data required as input is easier to obtain and thus often more readily available. To gain an uncertainty estimate for the tension-based groundwater recharge, we derived a range for the soil hydraulic model parameters based on measured texture (Section 2.1) using the pedotransfer function ROSETTA (Y. Zhang & Schaap, 2017), the average values are given in Table 3. This range only partly included the soil hydraulic model parameters as estimated from the undisturbed soil cores. As pedotransfer functions are considered to be location specific (Patil & Singh, 2016), we also included estimates for α, n and Ks using lookup tables from the German soil texture classification (Ad-hoc-AG Boden et al., 2005). Ranges for θ_s, α, n, and Ks are given in Table 3, θ_r and l were kept at the value determined in the evaporation experiment (0.069 cm^3 cm^{-3} and 0.5, respectively). With this, the same parameters are considered as in the uncertainty analysis for modeled groundwater recharge, but the likely range is kept considerably smaller than allowed in the optimization (see Table 1).

Different sets of soil hydraulic model parameters were derived by drawing 1,000 samples from their range using Latin Hypercube Sampling (McKay et al., 1979) that ensures that the parameter space is efficiently sampled, giving a comprehensive representation of the possible parameter combinations. The parameter sets were then

Table 4
Resulting Best Soil Hydraulic Model Parameters Using Different Soil Moisture Products as Target Variable in the Optimization

	Parameters	Units	SN	CO	WT	PC	MO
Plow layer (0–30 cm)	θ_s	cm^3 cm^{-3}	0.453	0.447	0.442	0.363	0.455
	α	cm^{-1}	0.0246	0.0442	0.0716	0.0033	0.0996
	n	-	1.31	1.13	1.23	1.26	1.18
	Ks	cm d^{-1}	32.26	83.87	66.7	6.66	66.7
Bottom layer (31–150 cm)	θ_s	cm^3 cm^{-3}	0.384	0.350	0.351	0.540	0.394
	α	cm^{-1}	0.0390	0.1000	0.0658	0.007	0.0284
	n	–	1.15	1.41	1.30	2.00	1.26
	Ks	cm d^{-1}	24.27	23.54	3.54	1.96	3.49

Note. For an explanation of model IDs see Table 2.

used to derive the tension-based groundwater recharge for the same time span as the modeled groundwater recharge.

3. Results

3.1. Calibrated Soil Hydraulic Models

The calibration using the different field-scale soil moisture products resulted in a good performance of the optimization (goodness-of-fit KGE at least 0.87 between measured and simulated variables). The variation in the goodness-of-fit measure between the 10 independent replications of the optimization were marginal (difference in KGE < 0.01), indicating the convergence and reliability of the optimization setup (Mai, 2023). This means that the independent optimizations result in equally valid parameter sets given the observed data. The one optimization with the highest KGE (even though only marginally superior) for each target variable (SN, CO, WT, PC, MO) is presented in the following as the best model (Table 4), while we also assess the effect of the equally valid parameter sets (Figure 2) on their ability to represent the root-zone soil moisture (Section 3.2) and on the resulting

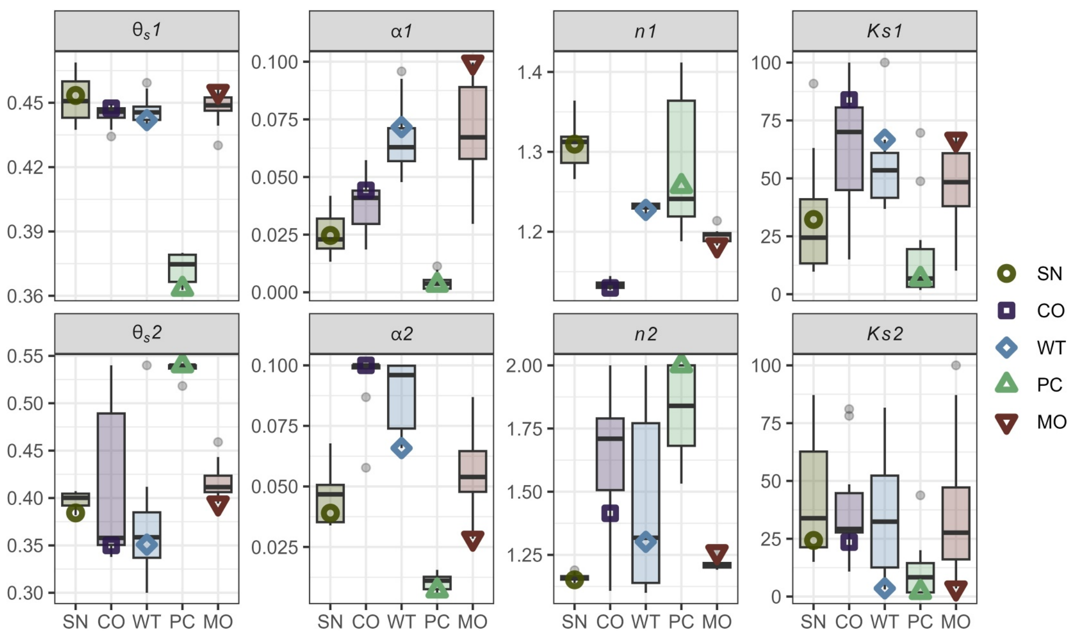

Figure 2. Distribution of the soil hydraulic model parameters from the repeated optimizations. The best model is marked with an according symbol. θ_s in cm^3 cm^{-3}; α in cm^{-1}; n (–) Ks in cm d^{-1}; the top row parameters indicated with 1 for the plow layer (0–30 cm), the bottom row parameters indicated with 2 for the bottom layer (31–150 cm).

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range in modeled groundwater recharge (Section 3.4). For most parameters, the optimum value is found within the specified parameter bounds (Table 1); only for CO, α in the bottom layer and for PC, θ_s and n in the bottom layer are touching the upper bound.

Figure 2 shows the parameter ranges for the repeated optimizations for each target variable (a full table of parameter values is provided in the data repository, see section Data availability). The parameter distributions confirm the non-uniqueness of the solution (equifinality) despite the narrow range in the objective function values between repeated optimizations. θ_s is well defined for the plow layer with a narrow range for all models and very similar median values for SN, CO, WT and MO. In the bottom layer this is only the case for SN and MO, while CO and WT show a larger range. Even with a small range PC shows a clear difference in θ_s compared to the other models. A similar behavior is observed for α, where PC has a small range, but much lower values than the other models. Considering SN to be the benchmark model, this clear deviation in several parameters calls for caution using PC. α values are high for the other models including CRNS data (CO, WT, MO), especially in the bottom layer. The parameter n is well defined (narrow range) in the plow layer, except for PC. In the bottom layer n shows a large spread especially for CO, WT and PC, while values are lower and well defined for SN and MO. Ks in both layers seems to be less identifiable, as the range obtained here is large, especially for the bottom layer, while PC again shows generally lower values than the other models. This larger spread is in line with findings from Brunetti et al. (2019), who also observed a higher uncertainty in defining Ks from inverse modeling. Soil hydraulic model parameters for MO are more similar to the models calibrated solely on CRNS (CO, WT) in the plow layer, and better resembling the median of soil hydraulic parameter distributions for SN in the bottom layer. For CO and WT, the parameters in the plow layer show a narrower range, while a large range for the bottom layer indicates the limited information content of the input data to constrain those. Overall, the parameter values for the benchmark model SN show a small range and thus its soil hydraulic model parameters are clearly defined.

3.2. Representation of Root Zone Soil Moisture

Figure 3 shows the modeled soil moisture of the baseline and SN model for the spin-up period (January to March 2013), the calibration period (April to July 2013) and the period of model application (August 2013 to March 2014) compared to the measured soil moisture θ_{SN}. It clearly shows that the calibration period covers the full range of measured soil moisture at the field site. With both the most pronounced dry phase and the strongest precipitation event occurring during the calibration period, we can expect the optimized soil hydraulic model parameters to be representative of the range of conditions and soil moisture stages observed at the field (Mertens et al., 2006). The baseline model using the initial parameter estimates follows the measured soil moisture dynamics with some offsets in absolute values and amplitude of dynamics, especially in the bottom layers, while a KGE of 0.72 suggests an acceptable performance for not having undergone calibration, a negative NSE and high RMSE and MAE indicate a need for calibrating the soil hydraulic model (Table 5). The calibrated model SN shows an improved match of simulated to observed soil moisture over the entire profile with a KGE 0.91. While the KGE is the optimization criteria the model is calibrated for, SN shows very good performance also for NSE, MAE, RMSE, and R^2 (Table 5). As the model is able to match the state variable over all depths down to 90 cm, we expect the model to represent water fluxes between layers equally well. This justifies SN to constitute a benchmark also in terms of downward flux passing the model boundary representing groundwater recharge at which to match the performance of the other models.

Figure 4 shows correlations of the simulated (using the best model) and observed soil moisture in all depths, together with the according RMSE values and the direct comparison to the baseline model. For SN, the calibration results in a better performance than the baseline model in all depths and the linear regressions (gray lines in the panels) are closer to the 1:1-line. For CO, an improvement over the baseline model is only evident in 10 cm depth with a clear offset of the linear regression to the 1:1-line and an underestimation of simulated soil moisture for the bottom layer. WT shows a clear improvement in the plow layer and only slight improvement in RMSE for the bottom layers compared to the baseline model. The overall performance measures for PC (Table 5) suggest a performance similar to the baseline model (some measures improve others get slightly worse). But Figure 4 shows that while the linear regression at intermediate depths (40–60 cm) are close to the 1:1-line, they cross the line for the plow layer and depths >60 cm and a worse performance in RMSE compared to the baseline is to be seen for the plow layer. This means while intermediate measured soil moistures are met in the simulation, low and high measured soil moisture values are over- and underestimated in the simulation, respectively. For MO on the other

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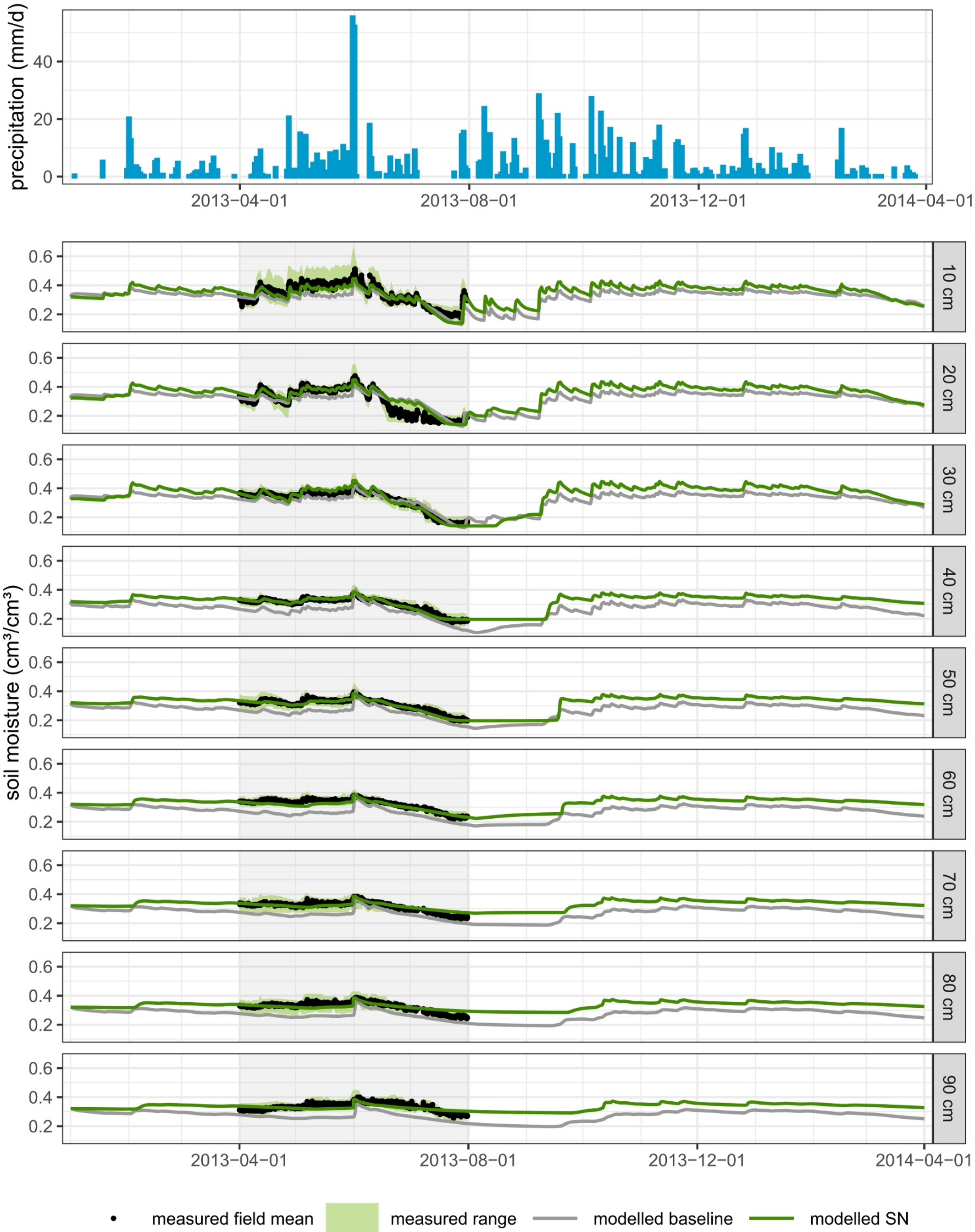

Figure 3. Daily precipitation (top panel) and soil moisture time series of the sensor network for its different measurement depths (bottom panels) as measured field mean (black dots, θ_{SN}) and the range from the 15 single sensor locations (light green area) and the soil moisture as simulated with HYDRUS 1D using the initial parameters (baseline, gray line) and the calibrated model SN (green line). The shaded gray area between April and August indicates the calibration time of 4 months.

hand, the RMSE in all depths is clearly improved over the baseline and the linear correlations are close to the 1:1-line.

Results for the best model realizations (Figure 4) are confirmed also for independently repeated optimizations and their equifinal solutions (Table 5). The ability to represent root zone soil moisture over the 90 cm depth is lower for models based solely on the CRNS information (CO and WT) as the median performance of both models shows values worse than the baseline model. The models combining CRNS and soil moisture profile information show a clear difference in their ability to represent root zone soil moisture. PC shows improved

Table 5
Performance Measures of Simulated Soil Moisture Compared to θ_{SN} for the Baseline Model and Calibrated Models Based on the Five Different Soil Moisture Products

		SN	CO	WT	PC	MO
	Baseline	Median (min, max)				
KGE	0.72	**0.91 (0.91, 0.92)**	−0.77 (−1.85, **0.85**)	0.28 (−1.36, **0.89**)	0.69 (0.54, **0.76**)	**0.90 (0.89, 0.90)**
NSE	−0.23	**0.83 (0.82, 0.83)**	−4.27 (−6.71, **0.21**)	−1.62 (−7.07, **0.81**)	**0.39** (−0.66, **0.49**)	**0.79 (0.77, 0.80)**
MAE	0.06	**0.02 (0.02, 0.02)**	0.12 (**0.04**, 0.14)	0.08 (**0.02**, 0.14)	**0.04** (**0.03**, 0.06)	**0.02 (0.02, 0.02)**
RMSE	0.06	**0.02 (0.02, 0.02)**	0.13 (**0.05**, 0.16)	0.09 (**0.03**, 0.16)	**0.04** (**0.04**, 0.07)	**0.03 (0.03, 0.03)**
R^2	0.67	**0.84 (0.83, 0.84)**	0.26 (0.21, 0.53)	0.51 (0.21, **0.81**)	0.48 (0.43, 0.60)	**0.81 (0.80, 0.81)**

Note. Given are the median, minimum and maximum value of the performance measures of the 10 repeated optimizations. Numbers in bold are an improvement over the baseline model.

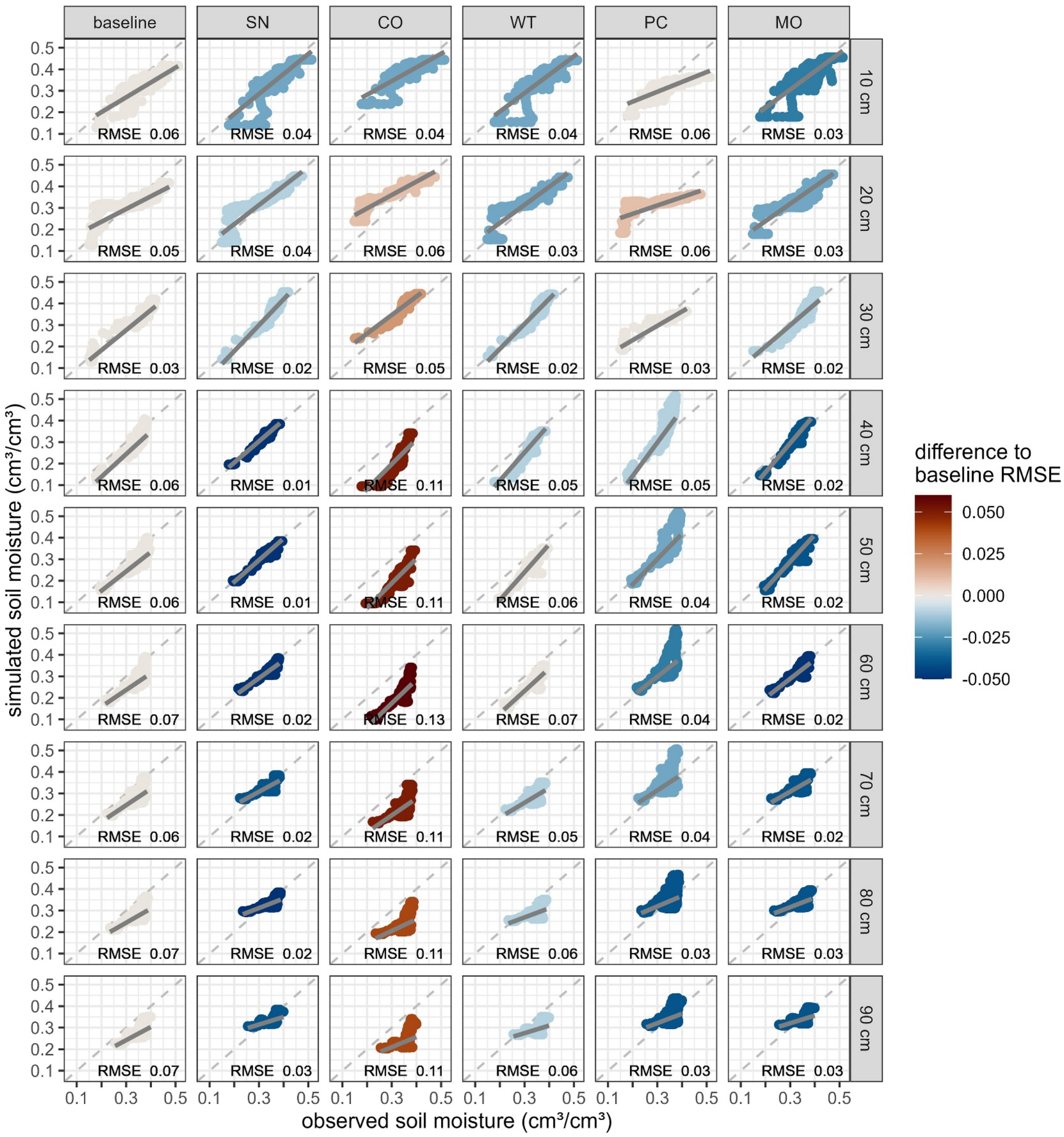

Figure 4. Scatterplot between simulated and observed soil moisture in all depths for the baseline and the five calibrated models. The numbers given in the plots are the root mean square error (RMSE), the solid gray line is the corresponding linear regression and the colors show the deviation to the RMSE of the baseline model with blue colors showing an improvement (decrease in RMSE) and orange colors indicating a deterioration (increased RMSE) compared to the baseline model. The gray dashed line is the 1:1-line.

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Table 6
Performance Measures of Simulated Soil Moisture Compared to θ_{SN} Considering Only Soil Moisture in the Plow Layer (0–30 cm)

	SN	CO	WT	
	Median (min, max)			SN(i)
KGE	0.92 (0.90, 0.93)	0.63 (0.61, 0.67)	0.92 (0.90, 0.92)	0.86 (0.79, 0.91)
NSE	0.84 (0.83, 0.85)	0.60 (0.53, 0.63)	0.85 (0.79, 0.86)	0.76 (0.48, 0.83)
MAE	0.02 (0.02, 0.02)	0.04 (0.04, 0.04)	0.02 (0.02, 0.03)	0.03 (0.02, 0.05)
RMSE	0.03 (0.03, 0.03)	0.05 (0.05, 0.05)	0.03 (0.03, 0.04)	0.04 (0.03, 0.06)
R^2	0.85 (0.85, 0.86)	0.86 (0.85, 0.86)	0.85 (0.81, 0.87)	0.83 (0.75, 0.85)

Note. Given are the median, minimum and maximum value of the performance measures of the 10 repeated optimizations for the models SN, CO, WT, and on single locations of the sensor network $SN_{(i)}$.

performance (median values) over the baseline model in NSE, MAE and RMSE, though not for KGE and R^2, while MO shows a clear improvement in all performance measures over the baseline model.

However, when focusing on the ability of the models to represent soil moisture in the plow layer (0–30 cm), the CRNS based models (CO and WT) achieve a much better performance (Table 6). Still, there is a clear difference and worse performance for CO compared to SN and WT. A decreasing fit of modeled to measured soil moisture over depth, when calibrating solely on neutron counts using the COSMIC operator is to be expected and was also found by Brunetti et al. (2019) and Barbosa et al. (2021). The higher median in all performance measures for WT opposed to $SN_{(i)}$ (Table 6) shows that each of the WT model replicates is able to match the observed field-scale soil moisture in the plow layer better than a model calibrated on single locations of the sensor network.

3.3. Seasonal Groundwater Recharge

During the calibration period, several precipitation events produce groundwater recharge as associated with a water outflow from the lower model boundary (bottom flux) at a depth of 150 cm depth (Figure 5). The intense precipitation event in May (two consecutive days >50 mm day^{-1}) promotes a substantial increase in groundwater recharge from the models. SN, CO, WT and MO show a more pronounced response to this event compared to the baseline and PC model, which show a dampened and temporally delayed response. In these models, simulated groundwater recharge after the calibration period persists to reach similar sums as SN after the calibration period, whereas no substantial recharge occurs in the other models after the calibration period until mid-October 2013. This dampened behavior compared to the other models is also pronounced during the main groundwater recharge period in winter and models result in distinct cumulative sums for one full year. PC (264 mm) and the baseline model (288 mm) result in lower sums than the other models with SN (333 mm), WT (333 mm) and MO (332 mm) reaching almost the same sum and CO (362 mm) the highest estimate. With this, the modeled groundwater recharge spans a range of approximately 100 mm.

Conversely, the tension-based water flux shows a more instant and pronounced response to precipitation. Especially for the strong precipitation event in May this effect in tension-based downward water flux is obvious, summing up to a cumulative flux of 193 mm over the consecutive 10 days, even exceeding the precipitation input of 108 mm. A comparable effect is visible during the winter recharge period. Consequently, the total groundwater recharge over the observation period was 688 mm (72% of precipitation) and substantially higher than the model estimates.

3.4. Uncertainty in Groundwater Recharge

As the 10 repeated optimizations for each target variable result in a range of soil hydraulic model parameters (Section 3.1, Figure 2) we assessed also the effect on the resulting groundwater recharge. Figure 6 (panel a) shows the ranges in cumulative groundwater recharge (for the simulated year) obtained from the equally valid model parameterizations. The good parameter constraint for SN results in a narrow range in groundwater recharge fluxes. Despite a wider spread in most soil hydraulic parameters for MO, the modeled groundwater recharge shows a similarly low variation as for SN. All optimizations for PC show the dampened behavior discussed before

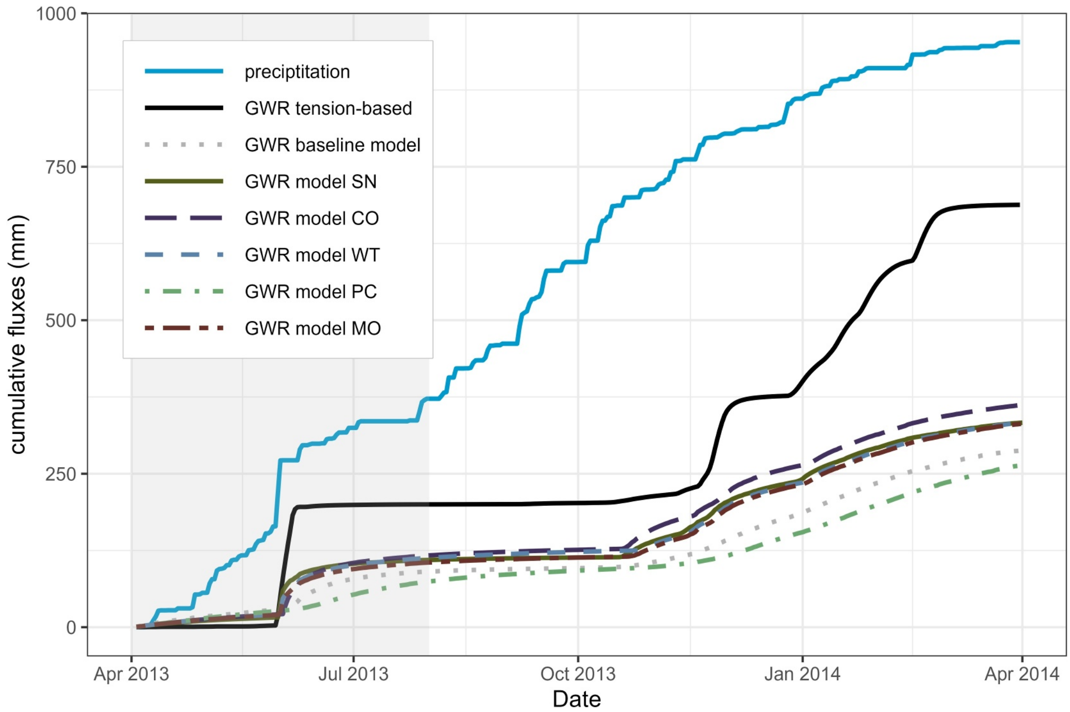

Figure 5. Cumulative precipitation and simulated cumulative groundwater recharge (GWR, mm) for 1 year, for the baseline and the five calibrated models (SN, CO, WT, PC, MO) as well as the tension-based groundwater recharge estimate (using the texture-based soil hydraulic model parameters, see Table 3). The shaded area marks the calibration period (1 April 2013 to 31 July 2013).

(Section 3.3) and result in lower cumulative groundwater recharge. For CO and WT a larger range and low outliers in the modeled groundwater recharge are to observe. Excluding those outliers, cumulative groundwater recharge at the end of the simulation period vary between 260 and 390 mm. This narrow range in modeled groundwater recharge is in line with findings of Jhorar et al. (2004), who found a good match of simulated water balance components despite a large spread in soil hydraulic parameters.

Considering the small-scale heterogeneity and variability in groundwater recharge associated with using individual locations of the sensor network as target variables, results in an increased range in annual cumulative groundwater recharge ($SN_{(i)}$, Figure 6, panel b) compared to the well constrained range in SN. Using single locations as a target variable next to CRNS soil moisture in $MO_{(i)}$ results in a range in cumulative groundwater recharge slightly narrower than the range for $SN_{(i)}$.

The overall uncertainty in modeled groundwater recharge can be assessed by the multi-model ensemble, consisting of the models calibrated on the different target variables, the independently repeated optimizations and using single locations of the sensor network instead of the field mean soil moisture profile. Figure 7, panel (a) shows the cumulative groundwater recharge from the multi-model ensemble (median 333 mm) compared to the groundwater recharge derived from soil water tension data (median 635 mm). While the tension-based groundwater recharge using soil hydraulic model parameters derived from texture information (Table 3) results in high groundwater recharge estimates (Figure 6, 72% of annual precipitation), the tension-based groundwater recharge using the soil hydraulic model parameters as derived from the laboratory experiment on the soil cores resulted in unrealistic high values (>2,000 mm), significantly exceeding the precipitation input. From the randomly sampled parameter sets used to derive an uncertainty estimate for the tension-based groundwater recharge, 11% of the parameter sets resulted in cumulative sums >2,000 mm. In panel (b) of Figure 7 the according ranges in soil hydraulic model parameters as used in the HYDRUS simulations and as applied for tension-based flux estimates are presented. Even though the range in soil hydraulic parameters for the tension-based groundwater recharge is much smaller compared to the values determined in the calibration over all models, the range in cumulative groundwater recharge from tensiometers is much larger. 30% of the tension-

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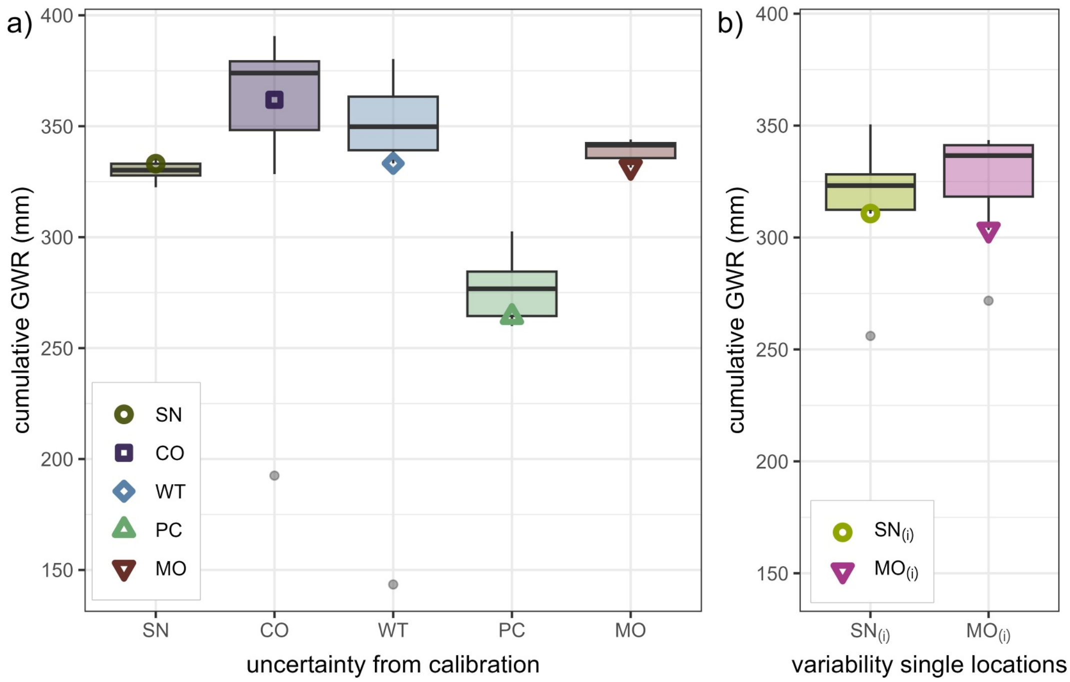

Figure 6. (a) Cumulative groundwater recharge (GWR) for the models SN, CO, WT; PC, MO and their corresponding 10 repeated optimizations with the resulting equally valid parameter sets. (b) cumulative groundwater recharge for models calibrated on single locations of the soil moisture sensor network SN(i) and a combination with CRNS soil moisture MO(i), representing the variability in groundwater recharge caused by small-scale heterogeneity in soil properties within the field site.

based groundwater recharge estimates exceed the annual precipitation input (953 mm) and 70% of the realizations exceed the highest simulated cumulative groundwater recharge from the models. However, its lowest values encompass the cumulative groundwater recharge from the models, which range from 31% to 40% of the annual precipitation.

4. Discussion

In the following, we first discuss the limitations in model setup and challenges from the model calibrations, then we discuss the main findings regarding the ability of the models to represent root zone soil moisture and provide consistent groundwater recharge, and finally we focus on the implications for using CRNS data to estimate groundwater recharge.

4.1. Model Calibration

For this study, the model setup was deliberately chosen to be simple, relying on daily input data of easy to obtain weather data (precipitation, minimum and maximum temperature). The aim is to evaluate a method that could be easily applied to other field sites, equipped with a CRNS and one or few additional point soil moisture sensors yielding profile information. The separation of the model domain into two soil layers was based on the available bulk density information, texture data alone could have allowed for a single layer system. This was regarded necessary after the first tests with a single layer system, where soil hydraulic model parameters in the optimization were touching the defined parameter bounds, indicating a non-optimal model setup (Mai, 2023). While a more complex model setup incorporating more processes (e.g., more detailed information on plant development and root water uptake) might lead to better results, usually they require additional parameters to calibrate in the model (Mertens et al., 2005; Wollschläger et al., 2009). Our parsimonious setup is found sufficient to evaluate the performance of using CRNS data compared to using soil moisture from an extensive sensor network. Lateral processes are considered to be of minor importance for the field site and can also not be represented by the HYDRUS 1D model. In case lateral processes are of importance, both methods for groundwater recharge estimation used in this study will fail.

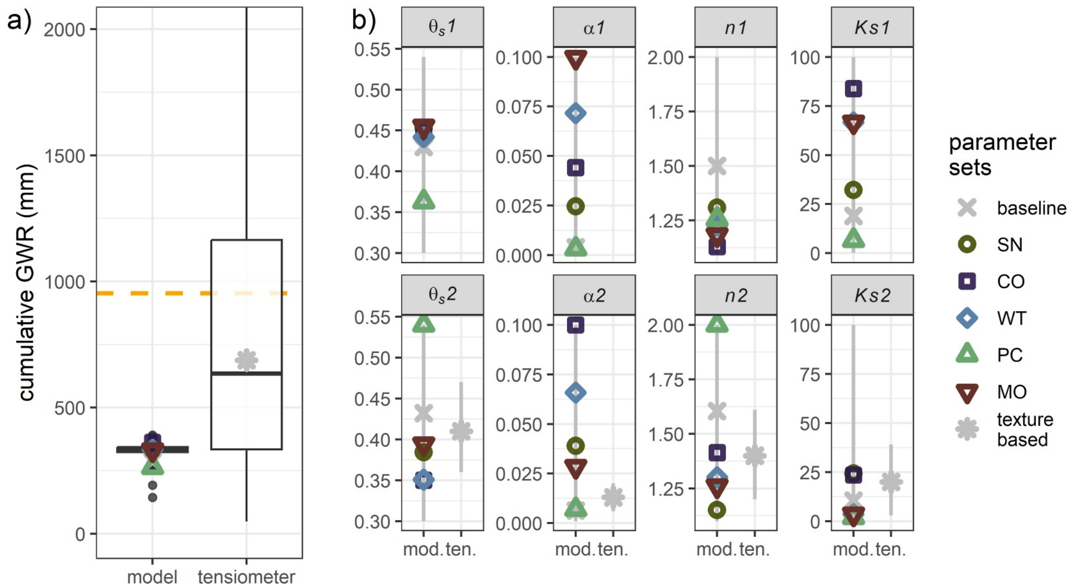

Figure 7. (a) Annual cumulative groundwater recharge (GWR) estimates from the multi-model ensemble and based on soil water tension data using different sets of soil hydraulic model parameters. The orange dashed line shows the annual precipitation input (953 mm). (b) The parameter ranges and best parameter set as resulting from model calibration, as well as the ranges in the parameters used to derive tension-based groundwater recharge (see Table 3). Soil hydraulic model parameters: θ_s in cm^3 cm^{-3}, α in cm^{-1}, n (−) Ks in cm d^{-1}, the top row parameters indicated with 1 for the plow layer (0–30 cm), the bottom row parameters indicated with 2 for the bottom layer (31–150 cm).

A successful model calibration depends amongst others on the appropriate range given for the parameter optimization (Mai, 2023). For soil hydraulic model parameters derived from inverse modeling using soil moisture data representative of large spatial scales however, it is important to emphasize their effective character. Studies have shown soil hydraulic model parameters derived on the lab-scale not to be transferable to larger scales (Mertens et al., 2005; Weber et al., 2024) and fail to reproduce soil hydraulic model parameters as derived in the field from paired tension and soil moisture measurements that are more appropriate to derive the fluxes in the field setting (Gribb et al., 2009). The effective parameters lose their physical meaning, the more they are of integrating nature (Mertens et al., 2005). The effective character of the often correlated soil hydraulic model parameters could also justify fixing more parameters to effectively calibrate the others, resulting in functional parameters with even less physical meaning (Pollacco et al., 2008). However, difficulties can arise on fixing parameters to the "correct" value (Foolad et al., 2017; Scharnagl et al., 2011).

Parameter bounds chosen in this study were wide, based on texture information and examples from literature and they allowed the optimization algorithm to find optimum soil hydraulic model parameters within the supplied range, using the sensor network data θ_{SN} in the resulting model SN and repeated optimizations. Also for the independent combination of θ_{CRNS} and few soil moisture profiles in MO, the optimum values of the soil hydraulic model parameters are found in the given range. Optimized parameters touching the bounds indicate issues to meet the target variable in inverse modeling. This is the case for CO and WT, where mainly parameters of the bottom layer are touching bounds (Figure 2), because the CRNS data (NC and θ_{CRNS}) does not contain information to constrain the parameters in this layer. Even though the soil moisture dynamics in deeper layers of the soil column depend on the soil moisture dynamics at the top, the soil hydraulic model parameters can vary more arbitrarily in this layer while still leading to a good performance in the objective function during calibration thus and increasing the equifinality of solutions. While θ_{CRNSpc} contains also information from point soil moisture and thus deeper layers in the soil column, its soil hydraulic model parameters tend also to touch the parameter bounds, especially notable for the high θ_s in the bottom layer. While the repeated optimizations show some parameters to be less well constrained (e.g., Ks, Figure 2), most parameters converge to similar values, confirming the robustness of the calibration. The differences between the parameter values then reflect the characteristics of the different soil moisture target variables, for example, the high dynamics in the top soil moisture from CRNS products, while θ_{CRNSpc} represents the more dampened average value of soil moisture in the profile.

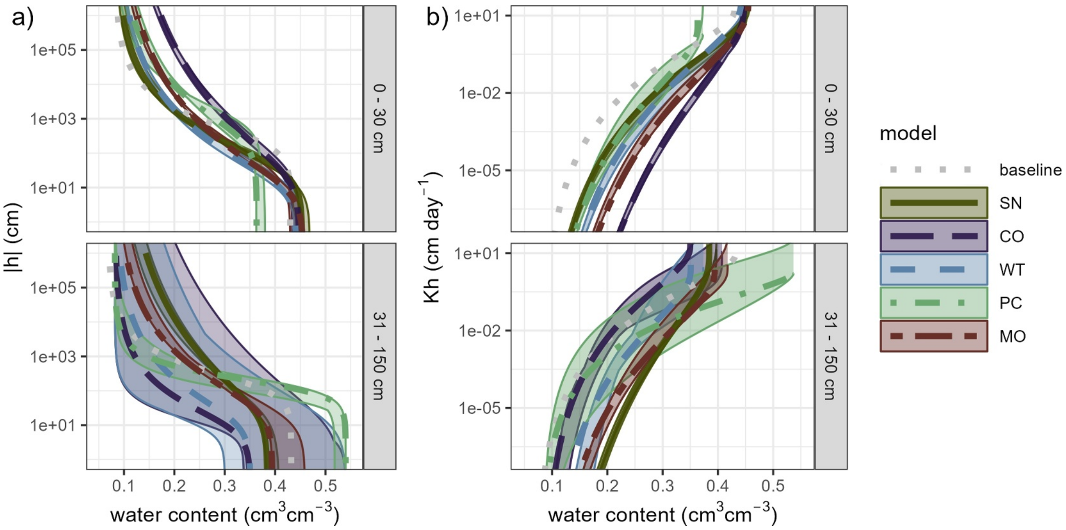

Figure 8. Soil hydraulic curves for the calibrated models and the according range from repeated optimizations. (a) Retention curve, (b) unsaturated hydraulic conductivity.

4.2. Soil Hydraulic Curves and Representation of Root Zone Soil Moisture

The calibrated models showed different ability to represent root zone soil moisture from a clear improvement to worse performance than the baseline model. While SN and MO show a high comparability over a range of performance measures and over all depths, CO and WT show high comparability only for the plow layer and lower comparability in deeper soil layers. PC shows an overall worse representation of root zone soil moisture than SN and MO, but more stable results than CO and WT for repeated optimizations. The correlation of simulated to observed soil moisture for PC shows the ability of the profile correction to represent average soil moisture conditions over the full soil profile (acceptable MAE and RMSE values, Table 5). However, the soil moisture dynamics are dampened (linear correlation crossing the 1:1-line, Figure 4), which also results in a dampened flux behavior in groundwater recharge.

The dampening effect of PC becomes obvious when comparing the soil hydraulic curves for the differently calibrated models. The shape of the retention function and unsaturated hydraulic conductivity of PC clearly deviates from the other models. The PC retention curve (Figure 8, panel a), especially in the bottom layer (31–150 cm), is much flatter than the curves of other models. In the bottom layer, this clear deviation is also to observe for the unsaturated hydraulic conductivity (panel b), for which PC shows a large range and lower conductivity for high soil moisture values.

The optimized parameters in the plow layer (0–30 cm) define the curve well, with larger ranges for all curves in the bottom layer, especially for CO and WT, showing the insufficient information content contained in their target variable to constrain the soil hydraulic model parameters in this layer. The curves for MO on the other hand match the benchmark model SN quite well for both, the retention curve and the unsaturated hydraulic conductivity in the plow as well as the bottom layer. The limited dynamics in the bottom layer result in a reduced range in soil moisture to estimate the soil hydraulic model parameters and consequently, the retention curve and unsaturated hydraulic conductivity curve tend to be steeper (for models with a good constraint in the bottom layer, i.e. SN and MO). This reduced soil moisture range might cause a bias for estimated soil hydraulic model parameters (Sonnleitner et al., 2003). For the retention curve and unsaturated hydraulic conductivity in the plow layer, a clear deviation between CO and WT is to observe, with WT better matching SN and thus explaining the improved ability to represent soil moisture in this layer. This could be caused by additional assumptions and parameters within the COSMIC operator, that are fixed in the current study before the optimization of soil hydraulic model parameters. The site specific scaling parameter N_{COSMIC} could either be calibrated as well, or the COSMIC operator itself could be improved to include more relevant neutron moderating factors, as shown by Iwema et al. (2021). While we assigned CRNS soil moisture in MO to be representative of a fixed integration depth (20 cm, see Table 2), the high performance of WT in representing soil moisture in the plow layer, indicate the high relevance of the vertical weighting. This might be even more important to consider for field sites with a larger range and deeper CRNS penetration depths. Additionally, the choice on how to weight the two target variables in the optimization of MO influences the result and should be reconsidered for the application of the approach at other study sites.

4.3. Groundwater Recharge Estimations

Notably, despite the wide range in soil hydraulic model parameters for calibrated models and in the differing ability to represent RZSM, cumulative GWR estimates from all models vary in a quite narrow range. As the sensor network used in this study is quite deep compared to other studies (e.g., Jakobi et al., 2018) and we are able to match measured soil moisture following model calibration in all depths, we expect the modeled flux for our benchmark case SN equally reliable. Already the uncalibrated baseline model shows groundwater recharge estimates similar to the estimates from the benchmark model. Despite the wide range in soil hydraulic model parameters and in the differing ability to represent root zone soil moisture, cumulative groundwater recharge estimates from most calibrated models vary in a quite narrow range compared to the estimates based on soil water tension. Cumulative groundwater recharge ranges obtained from repeated optimizations for CO and WT result in obvious outliers (Figure 6), stemming from the difficulty to constrain the soil hydraulic model parameters in the bottom layer using solely CRNS data for calibration (see Section 4.2) and giving a hint on an ill-posed calibration problem. However, the calibrated models match the measured soil moisture from the sensor network in the plow layer very well and outperform the use of a single location of the sensor network, which emphasizes their value to estimate field-scale parameters.

The models calibrated on CRNS data alone are able to meet the flux dynamics of the benchmark SN better than PC, implying that it is also essential to capture the higher dynamics of the plow layer, which are well represented by NC and θ_{CRNS} but not by the dampened signal of θ_{CRNSpc}. The high relevance of capturing soil moisture dynamics in the plow layer to achieve a representative flux separation in the physically based model might be location specific. We observe rather wet conditions throughout much of the cropping season with crop water requirements mainly provided from the plow layer, characterized by high root density. Soil water depletion of the bottom layer due to root water uptake is less pronounced but could be more important for other settings in determining the flux separation.

Using single locations of the sensor network for calibration ($SN_{(i)}$) results in a larger range in cumulative groundwater recharge than using the field mean profile (SN) (see Figure 6) giving an uncertainty estimate for the field-scale groundwater recharge. Compared to this uncertainty range, the majority of solely CRNS based models (CO and WT) result in rather high cumulative groundwater recharge estimates also exceeding this range, while groundwater recharge from MO shows high comparability to SN and also estimates from $MO_{(i)}$ stay within the range of $SN_{(i)}$. However, when considering a CRNS measurement setup to include only one soil moisture profile (setup as for $MO_{(i)}$), the data quality of this single profile is of large importance. In our calibration setup the depth specific soil moisture was decisive to calibrate the soil hydraulic model parameters for the bottom layer and while each of the model realizations of $MO_{(i)}$ are credible, the representativeness of the derived parameters is limited regarding their effective character. While we are able to derive effective hydraulic parameters for the plow layer using CRNS, larger uncertainty for estimating the bottom layer parameters can be assumed. If no soil moisture profile for deeper layers ia available, or the data are unreliable, a range for the parameters of the bottom layer could be achieved for example, from texture data and pedotransfer functions and performing a more thorough uncertainty analysis (e.g., in a Bayesian framework).

The comparison of modeled groundwater recharge to tension-based groundwater recharge confirms the timing of the model-based estimate. When a downward flux is calculated from the model, tension data indicates a downward flux, verifying the model results also beyond the calibration period. Variations in the soil hydraulic model parameters have shown to result in a very large spread in tension-based groundwater recharge, partially leading to estimates higher than the precipitation input. To consider here is the different scale and processes represented by the tension measurements (point-scale) and models (hectare-scale). Additionally, preferential flow or lateral processes not considered in the tension-based flux estimate might lead to locally high flux rates. This is again a consequence of small-scale heterogeneity and does not represent the behavior of the system at the field-scale. Modeled groundwater recharge rates, including the baseline model, are better comparable to estimates from other local studies (ranging from about 100 to 300 mm a^{-1} for the long term average, Neumann, 2005). Our results confirm the large benefit of using modeling and inverse model calibration to estimate effective soil hydraulic model parameters over direct measurements when targeting fluxes at the field scale (Ritter et al., 2003).

4.4. Benefits of CRNS Data in Groundwater Recharge Estimation

The simulation of the complex interactions between precipitation, evapotranspiration and groundwater recharge is enhanced by the integration of spatial and temporal information from measurements to estimate root zone soil moisture and groundwater recharge, the latter being often relevant on scales above the point-scale (i.e., at catchment or regional scales). The hectare-scale coverage of CRNS soil moisture with an integration depth substantially higher than remote sensing products enables the effective estimation of soil hydraulic model parameters and groundwater recharge in soil hydraulic models, as accurately as derived from an extensive sensor network. Sensor networks at agricultural sites are generally seldom available and especially for covering depths >50 cm. The sensor network used in the current study, covered only one vegetation period at the cropped field site because it conflicts with soil management operations, is such an exception. Permanent and long-term invasive sensor installations are usually found in grassland or forests (Bogena et al., 2013; Iwema et al., 2015), or not on the cropped field itself but on surrounding areas as grass strips (Heistermann et al., 2023; Schrön et al., 2017). The non-invasive nature of CRNS is advantageous in these settings, while still being representative for a large spatial footprint. CRNS can provide perennial soil moisture estimates also covering the major groundwater recharge period in winter. However, while the numerical simulation in HYDRUS 1D can include snow cover and infiltration or runoff from snow packs (Assefa & Woodbury, 2013), these periods might not be suitable for model calibration because of issues with the measured data. Dielectric sensors will not provide reliable soil moisture readings for frozen soil. Likewise, the water in snow cover will deteriorate the CRNS signal and comprise the soil moisture estimate, as no reliable distinction between their contributions to the signal can be made (Schattan et al., 2019).

Based on our results on using the CRNS data for calibrating a soil hydraulic model we can summarize recommendations, advantages and disadvantages:

- CO: using directly the measured neutron counts *NC*, which requires a minimal measurement effort and less preprocessing of the data, but on the other hand requires the use of a neutron transport approximation (e.g., the COSMIC operator). The latter necessarily comes with assumptions and increases the number of parameters to calibrate. An advantage for HYDRUS users is the existing implementation within the software allowing to also utilize the HYDRUS-internal calibration algorithms.
- WT: using the CRNS-derived soil moisture, which usually requires a soil moisture sampling campaign to relate the neutron counts to soil moisture, or as recently shown, can be derived using more easily available information on factors governing local neutron intensity (Heistermann et al., 2024). The use of a soil moisture for calibrating a soil hydrological model might be more intuitive to users and avoids the necessity of approximating neutron transport, which comes with its own uncertainty regarding parameters and process representation. The vertical integrated nature and inherent weighting of CNRS soil moisture θ_{CRNS} should be accounted for when comparing to depth specific simulated soil moisture, requiring an external calibration.

For both options, the depth representation of CRNS data is clearly a limitation and only the plow layer or a soil layer with a depth not exceeding the CRNS penetration depth should be calibrated, if no other information is available. If also data from soil moisture profiles is available, the model could be calibrated with the following calibration schemes:

- PC: using the soil moisture profile information to correct the CRNS-derived soil moisture. However, due to the dampened dynamics in θ_{CRNSpc}, this resulted in soil hydraulic model parameters more clearly deviating from our benchmark model and also in dampened water fluxes with quantitative estimates lower than SN, while still within a range observed from the spatial variability in the field $SN_{(i)}$.
- MO: using a multi-objective calibration based on CRNS soil moisture and soil moisture profile measurements. Effective soil hydraulic model parameters for the field scale were derived. However if only one soil moisture profile is available, the uncertainty on the model parameters in the bottom layer is critical.

While all the outlined approaches using the CRNS data for model calibration provide valid parameter sets, it is important to assess the uncertainty for the groundwater recharge estimate beyond the uncertainty stemming from the calibration procedure itself.

The results show CRNS to be suitable for calibrating a soil hydrologic model and derive groundwater recharge. Assuming the benchmark SN to represent the "true" hectare-scale groundwater recharge, also CRNS based model calibrations result in acceptable groundwater recharge estimates, even though precision and accuracy can be increased when additionally considering soil moisture from point-scale sensors for deeper depth as independent target variable in model calibration. The latter results in a model that allows at the same time to represent root zone soil moisture also in deeper depths. In drier regimes or at locations with fewer additional hydrogen pools, the effective penetration depth of CRNS is larger, but in general, the depth representativeness of the method is limited to the upper decimeters. Therefore, we strongly recommend augmenting CRNS field sites with one to three soil moisture profiles to gain insights into soil moisture dynamics of deeper layers. This allows to calibrate the soil hydraulic model parameters of these layers and results in better constrained flux estimates.

For comprehensive groundwater recharge estimation and the associated uncertainties in the amounts, incorporating multiple methods for groundwater recharge estimation at a single site, as suggested by studies like Scanlon et al. (2002) or Walker et al. (2019) is of great value and might even enhance the understanding of the system. We show that cosmic-ray measurements integrated in soil hydrological modeling can complement traditional hydrological methods for estimating groundwater recharge.

5. Conclusion

In this study, we conducted a comprehensive evaluation of calibrating a soil hydrologic model as implemented in HYDRUS 1D using different cosmic-ray neutron sensing (CRNS) soil moisture products. Using CRNS for model calibration results in accurate simulation of field-scale soil moisture within the shallow depth represented by CRNS, overcoming uncertainties linked to point-scale soil moisture data. However, relying solely on CRNS results in larger discrepancies in greater depths of the cropped root zone and consequently a larger spread in simulated groundwater recharge. This can be overcome by combining CRNS and point soil moisture data from deeper layers as independent target variables in model calibration, where already the use of one profile was sufficient to better constrain the soil hydraulic model parameters, resulting in consistent and realistic estimates for hectare-scale groundwater recharge. In contrast, groundwater recharge derived from soil water tension data solely captures the point scale and fails to sufficiently constrain plausible recharge rates using available information on the soil hydraulic model parameters. We strongly recommend augmenting CRNS sensors with at least one additional point sensor profile to derive soil moisture information beyond the CRNS penetration depth. This is particularly crucial when aiming to monitor not only shallow soil moisture and fluxes but also to extend the information to encompass the full root zone of a cropped field and target groundwater recharge effectively. We acknowledge that understanding the CRNS signal, including its integrating nature, the inherent weighting and variable penetration depth, may deter modelers from adopting CRNS soil moisture data. Nevertheless, our systematic assessment, conducted at the CRNS footprint scale, underscores the feasibility of integrating CRNS soil moisture data to enhance simulations of soil moisture states and essential water fluxes, including groundwater recharge.

Data Availability Statement

Most data for the field site is published within the BonaRes data set (Weber et al., 2021, 2022) at https://doi.org/10.20387/bonares-a0qc-46jc. Neutron count time series, calibration data from invasive soil sampling, as well as soil moisture time series from the sensor network can be obtained at https://doi.org/10.23728/b2share.8ab1022cc9f944108c540484f4f7be2d (Scheiffele et al., 2024). The repository also contains the files for the HYDRUS 1D model and a table with a complete set of soil hydraulic model parameters from the calibrations.

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