Improved representation of soil moisture processes through incorporation of cosmic-ray neutron count measurements in a large-scale hydrologic model

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Abstract. Profound knowledge of soil moisture and its variability plays a crucial role in hydrological modeling to support agricultural management, flood and drought monitoring and forecasting, and groundwater recharge estimation. Cosmic-ray neutron sensing (CRNS) has been recognized as a promising tool for soil moisture monitoring due to its hectare-scale footprint and decimeter-scale measurement depth. ~~Different approaches exist that could be the basis for incorporating CRNS data into distributed hydrologic models, but largely still need to be implemented, thoroughly compared, and tested across different soil and vegetation types~~But since CRNS provides an integral measurement over several soil horizons, a direct comparison of observed and simulated soil moisture products is not possible. This study establishes a framework to ~~accommodate neutron count measurements and~~ assess the accuracy of soil ~~water content~~ moisture simulated by the mesoscale Hydrological Model (mHM) by generating and comparing simulated neutron counts with observed neutron measurements for the first time. ~~It covers CRNS observations across different vegetation types in Germany ranging from agricultural areas to forest. We include two~~ We included three different approaches to estimate CRNS neutron counts in mHM ~~based on~~ as a function of the simulated soil moisture ~~: a method~~ profiles: two methods based on the Desilets equation and ~~another~~ one based on the forward operator COSMIC (Cosmic-ray Soil Moisture Interaction Code~~(COSMIC). Within the Desilets approach, we further test two different averaging methods for the vertically layered soil moisture , namely~~). For the Desilets method we tested two different approaches to average the vertical soil moisture profiles: a uniform vs. a non-uniform weighting scheme depending on the CRNS ~~penetrating depth. We use~~ measurement depth. The methods were tested at two agricultural sites, one pasture site, and one forest site in Germany. To explore the prior and posterior distributions of the mHM parameters when constrained by CRNS observations, we used a Monte Carlo ~~simulation method , specifically the~~ method based on Latin hypercube sampling ~~approach~~ with a large sample size (S = 100 000)~~to explore and constrain the (behavioral) mHM parameterizations against observed CRNS neutron counts. Overall, the three methods perform~~ . We found that all three methods performed well with Kling-Gupta efficiency ~~≥~~

~~0.8~~ > 0.75 and percent bias ~~< 1~~ $< \pm 10$ % across the majority of investigated sites ~~. We find that the~~ and for the best 1 % of parameter sets. The performance of the neutron forward models varied slightly across different land cover types. The non-uniform ~~weighting scheme in the Desilets method and COSMIC method provides the most reliable performance, whereas the more commonly used approach with uniformly weighted average soil moisture overestimates the observed CRNS neutron counts. We then also demonstrate the usefulness of incorporating~~ approach generally showed good performance, particularly at the agricultural sites. While the COSMIC method performed slightly better at the forest site. The uniform approach showed slightly better results at the grassland site. We also demonstrated for the first time that the incorporation of CRNS measurements into mHM ~~for the simulations of both~~could improve both, the soil moisture and ~~evapotranspiration and add a broader discussion~~ the evapotranspiration products of mHM. This suggests that CRNS is capable of improving the model parameter space in general and adds a broader perspective on the potential ~~and guidelines of incorporating CRNS measurements in~~ of CRNS to support large-scale hydrological and land surface models.

1 Introduction

Soil moisture is a key terrestrial climate variable because it controls the mass and energy exchange between the Earth's surface, the groundwater, the vegetation, and the atmosphere. Understanding soil moisture levels with changes in temperature is crucial for enhancing the predictability of climate patterns on inter-seasonal and annual time scales, as highlighted in previous studies (Santanello Jr et al., 2011; Seneviratne et al., 2006). Moreover, soil moisture variability also plays a significant role in a wide range of applications, including flood forecasting, weather forecasting, climate modeling, agricultural management, and groundwater recharge (Van Steenbergen and Willems, 2013; Albergel et al., 2010; Jablonowski, 2004; Wahbi et al., 2018; Samaniego et al., 2019; Barbosa et al., 2021). In hydrological modeling, soil moisture is a key variable controlling the partitioning of precipitation into evapotranspiration, infiltration, and runoff (Fuamba et al., 2019; Zhuo et al., 2020). Proper initialization and modeling of soil moisture are crucial for predicting other hydrologic processes (e.g., runoff, evapotranspiration, etc). Nevertheless, uncertainties in input data and model parameters, along with limitations in the representation of subsurface processes, can impede the reliability of soil moisture estimation (Chen et al., 2011). Obtaining accurate soil moisture measurements at a field scale is challenging due to current measurement limitations and subsurface complexity (Dong and Ochsner, 2018). Estimating average soil moisture at a mesoscale ($\approx$ 1–100 km) is particularly difficult due to measurement technique limitations in terms of their "footprint" and measurement methods to bridge the scale gap between point-scale and areal average measurements for hydrologic modeling (Chan et al., 2018).

One promising approach to infer soil moisture at a field scale is the cosmic-ray neutron sensing (CRNS) technique ~~(Zreda et al., 2008; De~~ (Zreda et al., 2008; Desilets et al., 2010; Zreda et al., 2012a). It is based on a neutron detector that counts the average number of neutrons in the air above the ground which represents the average hydrogen content in the environment. The method has demonstrated potential for estimating average soil moisture over areas of several hectares in size and tens of decimeters in-depth (Köhli et al., 2015; Schrön et al., 2017). CRNS probes are typically calibrated locally using soil samples within their support volume (Franz et al., 2012b; Schrön et al., 2017). CRNS data are used in various studies, including land surface modeling, vegetation dynamics, catchment hydrology, and supporting the agriculture sector with soil and climate data (Franz et al., 2020) . Moreover, CRNS derived soil moisture has been valuable in water balance studies, aiding in estimating infiltration and evapotranspiration (Schreiner-McGraw et al., 2015; Foolad et al., 2017; Wang et al., 2018).

When it comes to the comparison of observed CRNS soil moisture with the results from a hydrological model, a major challange is to select the right vertical scale. A CRNS measurement is an integral value over a measurement volume, and the depth of this volume depends on the soil moisture profile in a non-linear way (Köhli et al., 2015). While it is well understood in which depth the measured neutrons probed the soil, it is not directly clear how to compare the CRNS soil moisture product with several soil layers in a model. Shuttleworth et al. (2013) argued that the direct comparison of the raw product – the neutron counts – would be the favorable way to compare simulations with observations instead. By simulating neutrons directly, one could emulate the neutron counts per grid cell based on its soil moisture profile in the model, and then compare the result directly with the corresponding neutron measurement.

One way to calculate neutrons within the model is to use established empirical relationships between average soil moisture and neutrons (Desilets et al., 2010; Köhli et al., 2021). Another way is to employ the neutron forward operator COSMIC (Cosmic-ray Soil Moisture Interaction Code) introduces by (Shuttleworth et al., 2013). It emulates the effective vertical neutron transport through the soil and thereby enables a comprehensive representation of the neutron generation process. Although this operator can only be a simplification of the actual physical processes as modeled by, e.g., URANOS (Köhli et al., 2023), its higher complexity still comes with higher computational demand compared to the mentioned analytical relationships.

Previous studies, such as Barbosa et al. (2021) and Brunetti et al. (2019), have recognized the importance of CRNS over traditional invasive point-scale techniques and have utilized the HYDRUS-1D model to simulate soil moisture at the field scale. HYDRUS-1D offers a valuable framework for modeling soil moisture dynamics and has been particularly addressing the subsurface processes. ~~The~~ These studies incorporated a ~~COSMIC operator to simulate neutron count rates of a CRNS measurement (Shuttleworth et al., 2013)~~neutron forward operator COSMIC to simulate the neutron counts based on soil moisture profiles. They inversely calibrated soil hydraulic parameters by comparing observed and simulated neutron count rates, whereas beforehand this was limited to be done via comparison of depth-averaged soil moisture values (Rivera Villarreyes et al., 2014). The potential utility of using CRNS data to calculate volumetric soil water content (SWC) and improve soil hydraulic parameters within land surface models has also been observed earlier, as highlighted by Rosolem et al. (2014). ~~Furthermore, depth-weighting schemes and hydrogen pools' effects on measurement depth revealed valuable insights. Shallow wetting fronts in sandy soils significantly impact measurement depth Franz et al. (2012a). Baroni and Oswald (2015) assessed three weighting techniques, resulting in depths varying from 23 to 28 cm, optimal estimates were achieved using vertically varying weights and considering additional hydrogen pools.~~ In Iwema et al. (2017), a Land Surface Model investigated the impact of reducing scale mismatch between energy flux and soil moisture observations using CRNS data. Patil et al. (2021) employed a distributed Land Surface Model, Data Assimilation Research Testbed (DART) with CRNS time series, and Ensemble Adjustment Kalman Filter to simulate water and energy balance. Both studies focused on analyzing land surface water and energy balance, exploring data assimilation and calibration techniques.

The Hydrologiska Bryans Vattenbalansavdelning (HBV) model, as studied by Dimitrova-Petrova et al. (2020), employed CRNS data in a mixed-agricultural landscape to explore water balance on the land surface. While, Beck et al. (2021) used remote sensing products and groundwater level measurements to temporally calibrate the HBV model, emphasizing the challenge of comparing satellite-derived soil moisture with point-scale in-situ measurements. Additionally, Baatz et al. (2017) was the first study that utilized spatially distributed hydrological modeling, integrating CRNS data, FAO and BK50 soil maps, and other soil data in the Community Land Model (CLM). They demonstrated that assimilating CRNS data improved catchment-scale soil water content characterization by updating spatially distributed soil hydraulic parameters. Furthermore, Zhao et al. (2021) assessed the significance of CRNS data in CLM version 3.5, conducting simulations based on 13 CRNS stations over 2017-2018. Despite employing a simplified Richards equation, limitations included the absence of lateral flows and groundwater representation.

The mesoscale Hydrological Model (Samaniego et al., 2010b; Kumar et al., 2013b, mHM;) is known for its spatially distributed hydrologic predictions at a large scale incorporating ~~scale-aware regionalized parameterization technique. Therefore, by including a CRNS neutron count framework, the mHM model becomes a useful tool for improving simulated soil water content and furthering our understanding of the water cycle. This is made possible by the availability of observed CRNS data, which opens up new opportunities for research into novel hypotheses, improving model performance, and developing hydrological modeling methods.~~ with the multiscale parameter regionalization (MPR) technique. We chose the mHM in this study for its efficient parameterization approach that allows for a seamless prediction of water fluxes at different spatial resolutions (Samaniego et al., 2017; Zink et al., 2017; Jing et al., 2018; Schweppe et al., 2022). This feature allows the model to scale its applications from a locally relevant scale to regional and continental scales (Kumar et al., 2013b; Huang et al., 2017; Rakovec et . One of promising application of mHM is the operational German Drought Monitor (GDM) that provides daily updates on the soil moisture related drought status (Samaniego et al., 2013; Moravec et al., 2019; Pohl et al., 2023).Previous evaluation of the GDM for soil moisture focuses on assessing the skill of the model in reproducing SM anomalies based on point scale soil moisture observations(Zink et al., 2016, 2018; Rakovec et al., 2022; Scharnweber et al., 2020; Boeing et al., 2022). Such a evaluation is fraught with uncertainties due to scale mismatch between limited point scale observations versus grid-scale modeled estimates. In contrast, CRNS has been recognized as a promising tool for soil moisture monitoring due to its hectare-scale footprint and decimeter-scale measurement depth. Therefore, by including a CRNS neutron count framework within the mHM , it could better handle the scale mismatch issue and represent the soil moisture dynamics. The wide-spread availability of observed CRNS data opens up new opportunities to develop and implement novel methods and hypotheses to improve soil moisture representation in hydrologic models.

~~All the mentioned studies either compared the simulated and observed soil moisture products or incorporated the first COSMIC version to compare neutron counts directly.As argued by Shuttleworth et al. (2013), the usage of neutron counts is the favorable way to compare simulations with data, since the CRNS sensor intrinsically averages over soil moisture layers while the measurement depthvaries with soil moisture and consequently over time. Hence, the direct usage of CRNS neutron counts avoids the question of which modeled SWC layer the observations should be compared to and at what time scales. The~~

~~COSMIC method enables a comprehensive representation of the neutron generation process, which is computationally more demanding than using an analytical formulation (e.g., Desilets et al., 2010; Köhli et al., 2021).~~

In this study, we established a framework to incorporate CRNS data into the mesoscale Hydrological Model (mHM) to compare empirical and ~~physics-based~~ forward-modeling approaches for neutron count estimation to improve soil water content parameters in mHM across different vegetation types in Germany. To do this, we compared modelled with measured neutron counts to infer ~~soil hydraulic parameters~~optimal model parameters, such as soil hydraulic conductivity. Here, we test three approaches, (i) the direct calculation of neutrons from the equal-averaged SWC profiles based on Desilets et al. (2010), (ii) the same with ~~a~~ weighted-average ~~profile SWC~~ soil moisture profiles based on Schrön et al. (2017), and (iii) the ~~physics-based model~~ neutron forward operator COSMIC by Shuttleworth et al. (2013). We evaluate the simulation of neutron counts at scales of 1.2 km $\times$ 1.2 km, comparing the results to observed neutron counts from three different sites including agriculture, deciduous forests, and grasslands. The goal of this study is to investigate the potential of using CRNS probes and measured neutron counts to improve soil moisture predictions through simulations in mHM across different land covers and soil properties and to evaluate the feasibility of incorporating neutron count measurements into the modeling scheme. We employ a (calibration) framework by applying a Monte Carlo experiment to account for parameter uncertainties. We further cross-evaluate our simulations and test the reliability of the CRNS incorporated soil-moisture scheme in mHM for simulating other variables by utilising time series of observed evapotranspiration from an eddy covariance station available. Finally, we discuss and provide guidelines (challenges and limitations) for incorporating CRNS measurements in a large-scale hydrologic model. In summary, the present paper aims to answer the following research questions:

- What is the best approach to simulate CRNS neutron counts in a hydrological model considering the heterogeneity of vertical soil moisture profiles?
- What is the impact of model calibration with CRNS observations on simulated evapotranspiration at Hohes Holz?
- Is the mHM at approx. 1 km resolution capable of capturing the dynamics of hectare-scale CRNS measurements at different landcover sites in a grid including 2 agriculture sites, 1 forest site, and 1 meadow site?

2 Materials and Methods

2.1 Experimental Site Description

For this study, we select four sites with CRNS sensors, namely *Grosses Bruch*, *Hohes Holz*, *Hordorf*, and *Cunnersdorf* in Northern Germany, as provided already within COSMOS EU (Bogena et al., 2022) with particularly long time series and with different land cover, i.e., agriculture, forest, and meadow (see Tab. 1). The first three sites belong to the TERENO observatory "Harz/Central Germany lowland" (Zacharias et al., 2011) while the fourth site is part of an agricultural research farm operated by the German Weather Service (DWD). The *Grosses Bruch* site is a meadow/grassland that is usually flooded naturally once or twice a year. The meadows have sandy loam fluvisol-gleysol soil, which is 1.5 meters deep and partially covered with a layer of peat (Wollschläger et al., 2017). Meteorological conditions like soil moisture and temperature at various depths are continuously monitored by a wireless soil moisture monitoring network (Schrön, 2017). *Hohes Holz* is a deciduous forest site and the performance of the CRNS sensor there is highly dependent on dynamic effects such as tree canopy water or seasonal fluctuations in wet biomass. Water trapped in leaves and litter can present a particular challenge for CRNS measurements, especially at forest stations (Bogena et al., 2013). Also, Bogena et al. (2022) indicated that the influence of seasonal changes of biomass on the CRNS signal is much less important than the influence of changing soil moisture, even in ~~Hohes Holz~~*Hohes Holz*, as changes in soil moisture are the much larger source of variation represented by the CRNS measurements. The mean annual air temperature for each site ranges from 10.0 to 10.9 °C and the average yearly precipitation ranges from 458 to 535 mm.

Table 1. Geographical characteristics of study sites: Site Names, Geographic Coordinates, Climatic Data (Annual Precipitation in mm/year, Annual Mean Temperature in °C), and the Periods Covered in Observed and Simulated Datasets.

Site	**Latitude** [°N]	**Longitude** [°E]	**Altitude** [m]	**Land Cover**	**Precipitation** [mm/year]	**Temperature** [°C]	**Period**
Grosses Bruch	52.02	11.10	80	Pasture, grassland	458	10.1	24/06/2014–31/01/2021
Hohes Holz	52.09	11.22	217	Forest, hilltop	469	10.3	27/08/2014–31/01/2021
Hordorf	51.99	11.17	82	Cropland	463	10.3	29/09/2016–31/01/2021
Cunnersdorf	51.36	12.55	140	Cropland	535	10.9	23/06/2016–31/01/2021

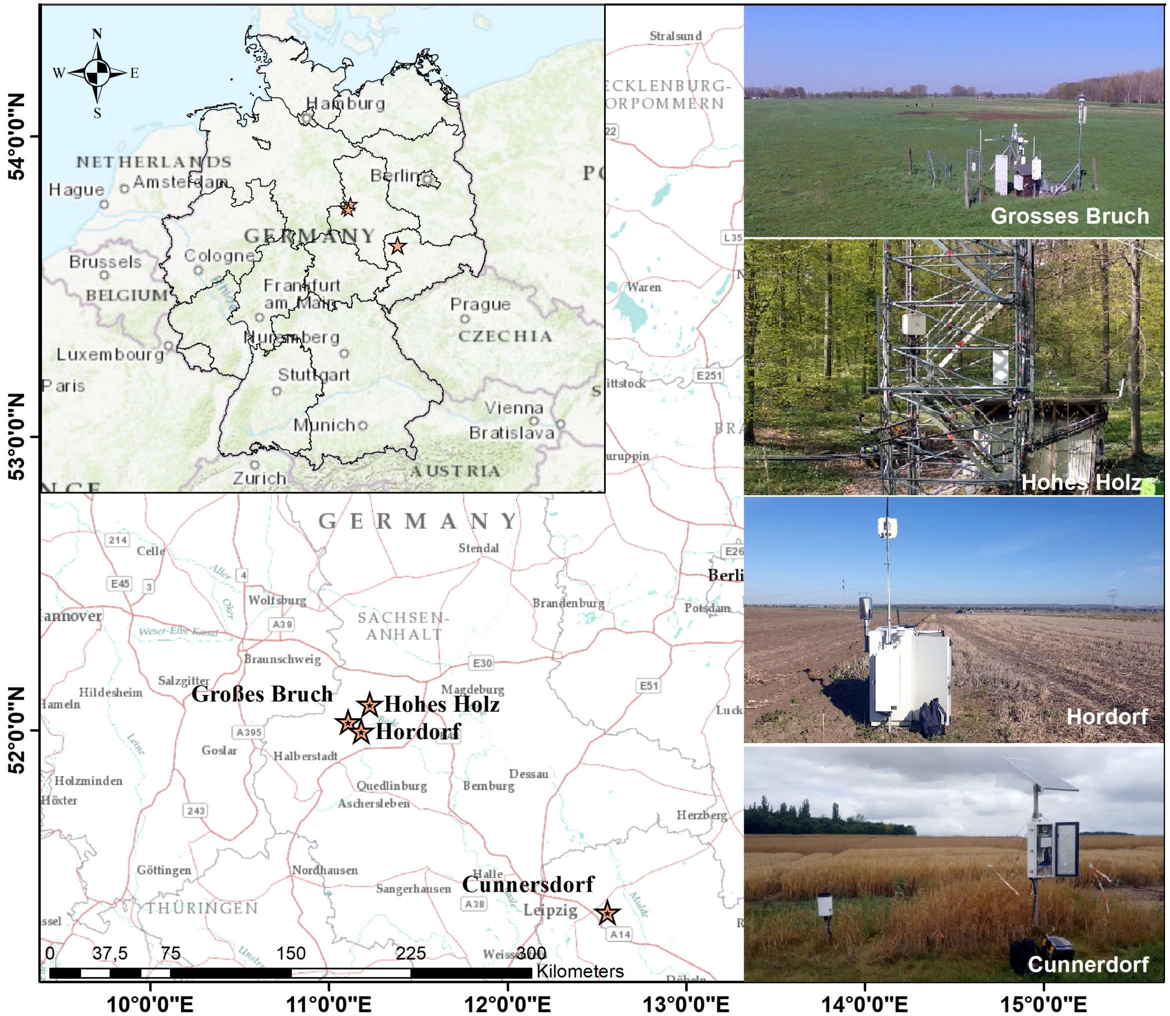

Figure 1. Study area map of Germany, highlighting the four test sites where observed neutron count rates from CRNS are utilized to evaluate the performance of mHM. The figure utilizes OSM basemap layers from (© OpenStreetMap contributors 2021; distributed under the Open Data Commons Open Database License (ODbL) v1.0) OpenStreetMap contributors (2020).

2.2 The mesoscale Hydrological Model (mHM)

mHM is a spatially distributed process-based hydrologic model ~~()~~ capable of representing processes such as canopy interception, snow accumulation and melting, soil moisture dynamics, infiltration and surface runoff, evaporation, underground storage, and runoff generation, deep infiltration and baseflow, as well as runoff attenuation and flood routing (Samaniego et al., 2010a; Kumar et al., 2013a). The mHM ~~model~~ is flexible for hydrological simulations at different spatial scales due to its novel Multi-scale Parameter Regionalization approach (MPR; Samaniego et al., 2010b); and has demonstrated applicability in diverse settings (Samaniego et al., 2010a; Kumar et al., 2013a; Rakovec et al., 2016a; Samaniego et al., 2017). The MPR's basic concept is to estimate parameters (e.g., porosity) based on soil properties (e.g., sand and clay content) using transfer functions at a fine spatial resolution (e.g. 100 m) and upscaling them to modelling resolutions (e.g., 1 km). In MPR, transfer functions (e.g., pedo-transfer functions to estimate soil parameters) are combined with morphological inputs (e.g., soil texture properties) and thus lead to model hydrologic parameters (e.g., porosity or hydraulic conductivity of the soil) (Livneh et al., 2015; Zacharias and Wessolek, 2007). In mHM, the soil moisture horizons/profile can be divided into several horizons, all of which are sensitive to root water uptake and evapotranspiration processes. mHM simulates the daily dynamics of soil moisture at different depths considering the incoming water (e.g., rainfall plus snow melt for the topmost layer and infiltration from above layers for other layers) and outgoing ET and ex-filtration fluxes. Further details on mHM code can be found at https://mhm-ufz.org~~and underlying modelling concepts at Samaniego et al. (2010a); Kumar et al. (2013a)~~.

2.3 Model Set-up

The latest version 5.12 of mHM is used in this study (see Samaniego et al., 2023, and https://github.com/mhm-ufz). The model ~~is executed over~~ was set up for a period of six years (2014–2020) with a daily time step, and the spatial resolution of the mHM grid cells ~~is fixed atL1 and L2: 0.01562° x 0.01562° is eq.~~was fixed at: $0.01562° \times 0.01562°$ ($\sim$ 1.2 km $\times$ 1.2 km using the WGS84 ~~Coordinate Systems.~~ coordinate systems). In mHM, Level 1 (L1) ~~describes~~ denotes the spatial resolution ~~, as~~ at which dominant hydrological processes are modelled and Level 2 (L2) ~~describes~~ denotes the resolution of the meteorological forcing data. The finest resolved spatial level L0 ~~: 0.001953125° × 0.001953125°. Level 0 (L0) describes~~ ($0.001953125° \times 0.001953125°$) denotes the subgrid variability of relevant basin characteristics, which includes information on the soil as well as land use, topography, and geology.

Figure 2 shows the flow diagram depicting the basic methodology of our study, which includes the calculation of CRNS neutron count rates based on daily soil moisture values simulated with mHM. The model boundary conditions such as precipitation and temperature for the mHM ~~model~~ are acquired from the German Weather Service (DWD) station closest to the test site. The potential evapotranspiration required by mHM is estimated using the Hargreaves-Samani method (Hargreaves and Samani, 1985). The model setup and parameterization for the soil moisture module use the scheme optimized by Boeing et al. (2022). A raster dataset describing the distribution of the soils in the model area and a corresponding lookup table with the attributes depth, soil texture (sand and clay fraction), and bulk density are required as soil input data and are derived from national digital soil maps provided by the Federal Institute for Geosciences and Natural Resources (BGR, 2020). The data set contains physical and chemical properties for soil at different layers and the available at a resolution of 1:250,000 (BUEK 200; BGR, 2020). mHM uses three dominant land cover classes (forest, permeable, and impervious) that were retrieved by a GLOBCOVER database ESA (2009). Furthermore, vegetation characteristics like Leaf Area Index (LAI) and fraction of roots for different vegetation types are prescribed in the model. The mHM soil domain is divided into three horizons with depths of 0–5 cm, 5–25 cm, and 25–60 cm. The upper two model layers are parameterized using the topsoil layer properties while for the lower model layer, the subsoil properties are used. More details on the underlying input data for mHM can be obtained from Boeing et al. (2022).

In our study, we utilized three distinct modules of parameters: ~~Snow, Soil Moisture, and Neutrons~~snow, soil moisture, and neutrons, with a total of ~~29~~ 28 parameters employed for the Desilets method and ~~31~~ 30 parameters for the COSMIC method. The simulation of soil water content is processed through these three modules to estimate neutron counts. To comprehensively cover the parameter set ranges, we employed 100 000 iterations. Finally, we selected the top 10 optimized parameter sets based on the objective function, $KGE_{\alpha\beta}$, for further analysis and evaluation.

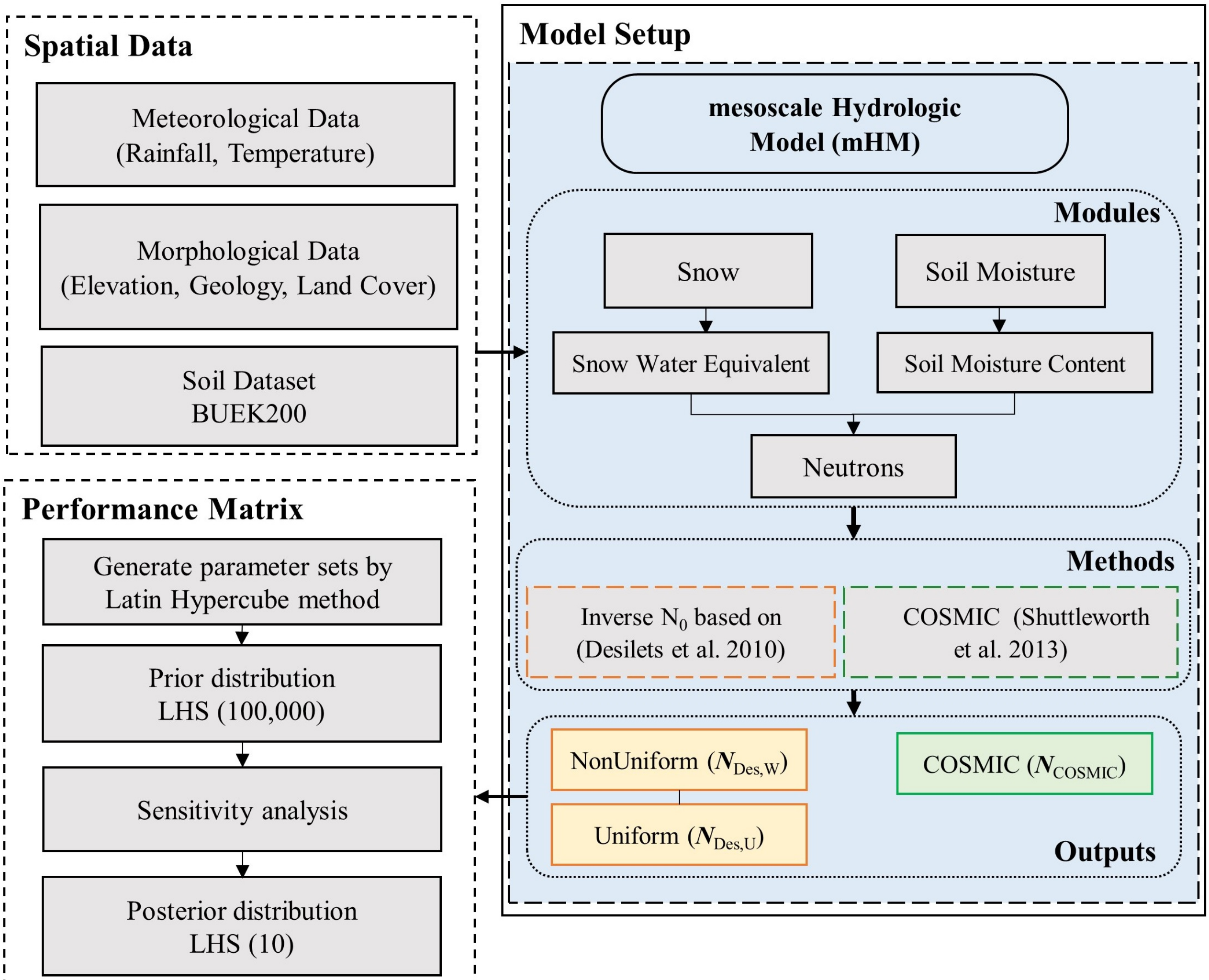

Figure 2. Flowchart depicting the methodology employed for calculating CRNS neutron counts through the utilization of the LHS technique for parameterization in mHM. The computation of CRNS neutron count is carried out through three distinct approaches: $N_{\mathrm{Des,U}}$,$N_{\mathrm{Des,W}}$, and N_{COSMIC}.

2.4 Conversion of soil moisture to neutron count rate

In this study, we ~~compare~~ compared observed neutron counts from CRNS data with simulated neutron counts estimated from modeled soil moisture with the goal of optimizing the parameterization of soil water content from mHM shown in Fig. 3. By ~~coupling~~ incorporating the approaches from Desilets et al. (2010) and Shuttleworth et al. (2013) ~~each directly with the mHM model~~directly into the mHM , we are able to account also for the uncertainty in the model predictions and test their feasibility across four distinct sites. We analyzed the soil water content data at different soil layers (0–5 cm, 5-25 cm, and 25-60 cm) in mHM, as utilized in the study by Boeing et al. (2022). The accuracy of numerical calculations ~~(such as Shuttleworth et al. (2013) set up)~~ would benefit from higher resolved soil profiles, however, our experiments demonstrated that varying soil depths from 3 to 6 layers did not have a substantial impact on the simulated neutron count results in mHM. We used BGR (2020) which is a global dataset that is not detailed enough to allow for finer vertical resolution. Our main objective is to optimize the parameterization of soil hydraulic properties in mHM based on the comparison between measurement and modelled neutron counts.

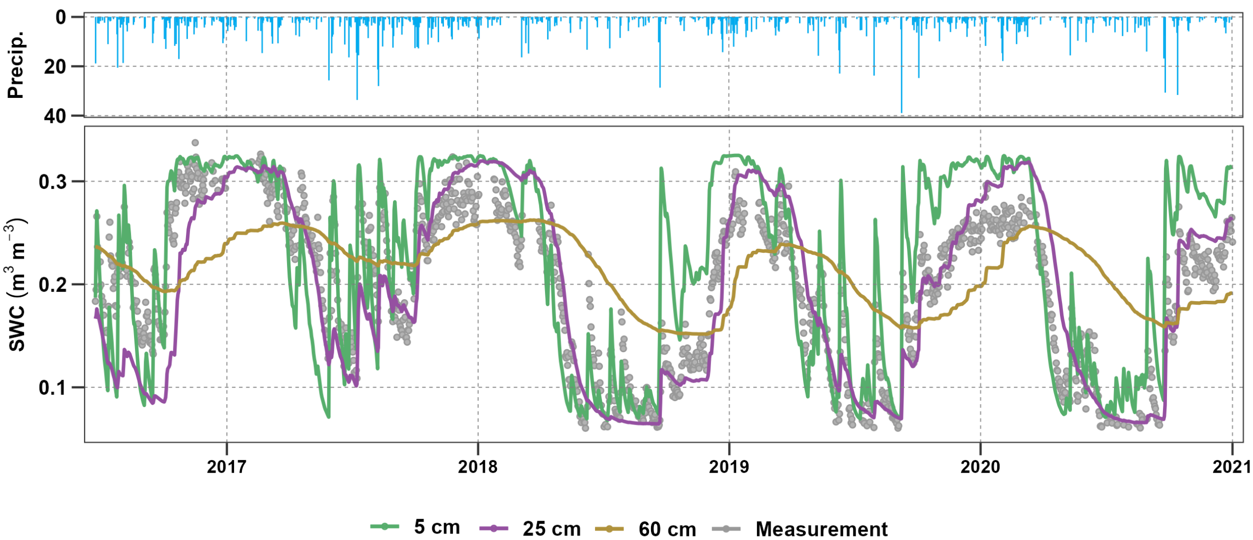

Figure 3. Daily time series of soil water content (cm^{3}cm^{-3}) at the *Cunnersdorf* site. The graph shows a comparison between the measured SWC from CRNS data representing an integral over the first decimeters and the simulated data derived from the mHM for three distinct soil depths, at 0–5 cm (green), 5–25 cm (purple), and 25–60 cm (brown).

2.4.1 Desilets based method

In the present study, we utilize the soil moisture information from the mHM ~~model~~ to convert it into neutron counts using the ~~Desilets et al. (2010)~~ empirical-based approach by ~~calculating neutron counts from soil moisture, three constant parameters~~Desilets et al. (2 . ~~which is further improved by adding~~ We also added lattice water and bulk density ~~following the approaches by~~ information following the suggestions from Dong et al. (2014) and Hawdon et al. (2014), respectively. ~~Theoretically, the N_0 parameter~~ This empirical approach makes use of a free scaling parameter N_0, which represents the neutron count rate ~~level of the~~ of a particular CRNS probe ~~used for rather dry soil at the local conditions, should be~~ under dry soil conditions. This parameter is typically site-specific but does not change over time, as noted by Franz et al. (2013) and Hawdon et al. (2014). ~~In order to obtain accurate measurements of soil moisture using CRNS data in the mHM model, N_0 has to be estimated through calibration and is crucial as it directly affects the accuracy of the mHM neutron counts results. This calibration parameter is specific to each site environment and reference condition. This parameter primarily depends on site-specific environmental factors and reference conditions. This coefficient is specific to~~ It is also specific to the particular CRNS detector and may be ~~impacted~~ influenced by factors such as terrain (topography)~~but also~~, local soil, vegetation characteristics, and additional hydrogen pools (e.g., from organic ~~material~~matter) at each observation site~~Schrön et al. (2021)~~. Therefore, ~~calibration~~ the determination of N_0 ~~is necessary for each CRNS data set at a site to ensure realistic model output. Neutrons are sensitive to all kinds of hydrogen in the footprint, hence the variable θ denotes not only soil moisture, θ_{sm}, but is rather assumed to also include lattice water, θ_{lw}, as well as water equivalent from soil organic carbon, θ_{org}, and vegetation biomass, θ_{bio}~~by local soil sampling campaigns is necessary. Once determined, , the parameter N_0 should be kept constant or carefully calibrated within limits of not more than $\pm5\%$. As a sensitive parameter, N_0 strongly influences the accuracy of the mHM soil moisture results.

Soil moisture for three vertical mHM soil layers is used ~~to drive~~ as input for both the Desilets method and the COSMIC operator. To improve comparability between measurements and modeling techniques, Schrön et al. (2017) ~~propose the depth-weighted approach~~proposed to weight the soil moisture values of each layer by their depth. This approach ~~incorporates the contributions of different soil layers by calculating~~ results in a depth-weighted average SWC, θ_{avg} ~~, resulting in a more comprehensive representation of soil moisture dynamics. This gives CRNS neutron count rates, after being corrected for incoming neutron flux, pressure, and air humidity variations, to be~~ that better represents the complex behaviour of neutrons to probe the soil.

$$N_{\text{Des}} = N_{0,\text{Des}}\left(\frac{a_0}{(\theta_{\text{avg}}+\theta_{\text{lw}})/(\varrho_b/\varrho_w)+a_2}+a_1\right) \qquad (1)$$

Among the four parameters, ~~three of which are coefficients parameters a_i~~ $a_{0...2}$ were determined empirically by ~~(Desilets et al., 2010) who~~ Desilets et al. (2010). The authors derived $a_0 = 0.0808$, $a_1 = 0.372$, and $a_2 = 0.115$ ~~, and are considered as constants for values of~~ for $\theta > 0.02\, gg^{-1}$. The fourth parameter, $N_{0,Des}$ is ~~N_0 when using the Desilet's equation, and here is a free calibration parameter. Whereas the parameter~~ fixed based on field measurements, with its value taken from Bogena et al. (2021). Since neutrons are sensitive to all kinds of hydrogen in the footprint, the variable θ denotes not only soil moisture, it is rather assumed to also include lattice water, θ_{lw}, as well as water equivalent from soil organic carbon and vegetation biomass. More precisely, θ_{lw} is the grid average volumetric water content of the equivalent lattice water content of the CRNS area (cm^3 cm^{-3}), ϱ_b (g cm^{-3}) is the bulk density of the dry soil, usually determined from soil samples, and ϱ_w = 1 g cm^{-3} is the density of water. Regarding the variables of Soil Organic Carbon (SOC) and biomass, it's important to note that these variables are often not readily available, especially when it comes to biomass data. ~~To address this, the free parameter N_0 is utilized to account for~~

~~these unknowns.~~ For lattice water, we assume a linear relationship to clay content (Avery et al., 2016):

$$\theta_{\mathrm{lw}} = \theta_{\mathrm{lw0}} \cdot C + \theta_{\mathrm{lw1}}\,, \tag{2}$$

C denotes the clay fraction in % (Greacen, 1981). The derived quantity lattice water, θ_{lw}, is regionalized based on C and varies between 0.0 and 0.1 $\mathrm{m}^3/\mathrm{m}^3$. In order to obtain the average soil moisture for a layered soil moisture profile within mHM, the following averaging equation is employed:

$$\theta_{\mathrm{avg}}(w,\theta) = \frac{\sum_{i=1}^{n} w_i\,\theta_i}{\sum_{i=1}^{n} w_i} \tag{3}$$

where the volumetric soil water content at a specific layer of mHM in a given profile is denoted by θ_i ($\mathrm{m}^3\ \mathrm{m}^{-3}$). The total number of layers in all soil sampling profiles is represented by the variable n, and the weight assigned to layer i is denoted by w_i. In the uniformly weighted approach, all weights equal one:

$$N_{\mathrm{Des,U}} = N_{\mathrm{Des}}(w_i = 1) \quad \forall i\,. \tag{4}$$

In the weighted-averaging approach, the weights are determined based on Schrön et al. (2017):

$$N_{\mathrm{Des,W}} = N_{\mathrm{Des}}(\theta_{\mathrm{avg}}(w,\theta))\,, \tag{5}$$

$$\text{where} \quad w_i = \int_{z_{i,\mathrm{min}}}^{z_{i,\mathrm{max}}} e^{-2\,z/D}\,\mathrm{d}z \propto e^{-2\,z_{i,\mathrm{min}}/D} - e^{-2\,z_{i,\mathrm{max}}/D}$$

$$\text{and} \quad D = \varrho_b^{-1}\left(p_0 + p_1\left(p_2 + \mathrm{e}^{-p_3\,r}\right)\frac{p_4+\theta}{p_5+\theta}\right). \tag{6}$$

Here, the integral goes through each horizon from $z_{i,\mathrm{min}}$ to $z_{i,\mathrm{max}}$ in 1 mm steps and sums up the weight over the whole layer. z_i is the depth of the given soil moisture layer i, D is the average vertical footprint depth of the neutrons, p_i are numerical parameters presented in Schrön et al. (2017), and r (m) represents the distance from the sensor. It should be noted that the equation for D is valid for $\varrho_b > 1.0\,\mathrm{g\,cm^{-3}}$ and soil moisture contents above $\theta > 2\,\%$ ~~Kasner et al. (2022)~~(Kasner et al., 2022) . In our model, we set $r = 1$ m which is sufficient to represent the average depth across the footprint radius within the model grid. The soil moisture profile is converted to a single average neutron count per grid cell using Eqs. 1–5.

2.4.2 Cosmic Ray Soil Moisture Interaction Code (COSMIC)

The Cosmic Ray Soil Moisture Interaction Code (COSMIC) is an ~~analytical, physics-based model that is well-suited~~ neutron forward operator that has been developed for data assimilation applications ~~. It includes descriptions of the degradation of~~ (Shuttleworth et al., 2013). The model aims at mimicing the physical processes of neutron transport in the vertical dimension of the soil using a simplified analytical formulation of the most relevant mechanisms and their effective parameterizations. Shuttleworth et al. (2013) reported that this lack of complexity might introduce systematic errors for typical soil moisture profiles on the order of 2 % compared to physics-based models (e.g., Köhli et al., 2023). However, the simplified approach allows to estimate neutron counts with a computational efficiency that is several orders of magnitude faster.

The COSMIC model assumes a downwards attenuation of incoming high-energy ~~neutron flux~~ neutrons with soil depth, the production of fast neutrons ~~at each soil depth, and the scattering of resulting fast flux neutrons before reaching the soil surface~~in each soil layer, and an isotropic scattering of the resulting fast neutrons that is projected upwards. These processes ~~have a parametric dependence on soil chemistry and moisture content . The COSMIC method solves this inverse problem by calculating neutron count rate based on soil water profiles, which could then be compared with observed neutrons without the need to deal with dynamic sensing depths or weightings.~~

exhibit a parametric dependency on soil properties and water content and lead to a resulting neutron count value for each grid cell in mHM.

$$N_{\text{COSMIC}} = N_{0,\text{COSMIC}} \sum A_{\text{high}}(z) X_{\text{eff}}(z) A_{\text{fast}}(z)\,, \tag{7}$$

where $\quad A_{\text{high}}(z) = e^{-\Lambda_{\text{high}}(z)}\,,$

$$A_{\text{fast}}(z) = \frac{2}{\pi} \int\limits_0^{\pi/2} e^{-\Lambda_{\text{fast}}(z)} (\cos\varphi)^{-1}\,\mathrm{d}\varphi\,,$$

$$X_{\text{eff}}(z) = \alpha_{\text{COSMIC}}\, X_{\text{soil}} + X_{\text{water}}\,.$$

~~In this model ,~~ We used soil samples from the COSMOS-Europe paper (Bogena et al., 2022) to run the COSMIC model in order to determine the scaling factor $N_{0,\text{COSMIC}}$, following the established strategies (Shuttleworth et al., 2013; Patil et al., 2021; Baatz et al. . In Eq. 7, A_{high} represents the high-energy neutron attenuation, A_{fast} represents the fast neutron attenuation, and X_{eff} represents the production of fast neutrons from high-energy neutrons ~~in the soil-water composite~~at any level in the soil. It takes into account the different mechanisms in both, water and soil, where the soil is typically less effective in producing fast neutrons by a factor of $\alpha_{\text{COSMIC}} \approx 0.24$ (g cm^{3}g^{-1}), depending on bulk density.

$$X_{\text{soil}}(z) = \Delta z \varrho_{\text{b}}\,, \tag{8}$$

$$X_{\text{water}}(z) = \Delta z \varrho_{\text{water}}(\theta_z + \theta_{\text{lw}})\,, \tag{9}$$

The ~~total attenuation lengths of high~~ effective attenuation of high-energy and fast neutrons in the ~~soil water~~ soil-water composite are described ~~using physically motivated~~ by physically motivated functional relationships with effective length scales L_i.

$$\Lambda_{\text{high}}(z) = \frac{X_{\text{soil}}(z)}{L_1} + \frac{X_{\text{water}}(z)}{L_2}\,, \tag{10}$$

$$\Lambda_{\text{fast}}(z) = \frac{X_{\text{soil}}(z)}{L_3} + \frac{X_{\text{water}}(z)}{L_4}\,. \tag{11}$$

The ~~COSMIC function considers the attenuation of incoming high-energy neutrons (A_{high}) and their interaction with soil to produce effective neutrons (X_{eff}) in addition to the attenuation of isotropically propagating fast neutrons. The parameter α_{COSMIC} represents the soil's relative efficiency of forming fast neutrons, and~~ length constants L_1, L_2, L_3, and L_4 (in g cm^{-2}) are related to local soil properties. COSMIC uses several time-invariant, site-independent, and site-specific parameters, including L_1 = 162.0 (g cm^{-2}), L_2 = 129.1 (g cm^{-2}), and L_4 = 3.16 (g cm^{-2}), as reported by Shuttleworth et al. (2013), regardless of location. However, the L_3 (g cm^{-2}) parameter ~~vary~~ varies with soil bulk density ϱ_b which may change with depth. ~~The parameter L_3 is correlated with the soil bulk density and according to the model code,~~ In mHM, this is expressed by a linear relationship of regionalized parameters L_{30} and L_{31} ~~nomenclature are given as per the model code in mHM ().~~ :

$$L_3 = L_{30}\varrho_\mathrm{b} - L_{31}. \tag{12}$$

The ~~regional~~ original formulation of the COSMIC method has been ~~revised to include the θ_lw~~ further extended by the inclusion of layer-wise lattice water content ~~as well.~~

~~Besides the addition of lattice water to the code, the original version of COSMIC has also~~ and bulk density. Furthermore, COSMIC inside mHM has been numerically optimized to substantially increase the computational performance. This includes the calculation of the ~~geometric~~ projected integral (Eq. 7) based on lookup tables.

2.5 Constraining of model parameterization

In this study, we employ a model calibration technique to identify the most suitable parameter values for the mHM ~~model~~. Specifically, we utilize a total of ~~29~~ 28 parameters for the Desilets based method and ~~31~~ 30 parameters for the COSMIC method which includes hydrologic processes related to: snow, soil moisture, and neutron counts dynamics. The process of model calibration involves modifying the parameter values of the model to achieve a satisfactory standard for an objective function by comparing the predicted output with the observed data (James, 1982). We use the general concept of the KGE as a weighted combination of the three components (bias, variability, and correlation terms) to evaluate our simulation (Gupta et al., 2009). We excluded the correlation component from ~~(Eq. ??)~~ (Gupta et al., 2009) equation as our simulation already exhibited satisfactory correlation due to strong seasonality, we opted not to consider it in our assessment (objective function), as it accounted for 33% of the total weighting in the overall KGE score. Seasonality is an inherent characteristic in the northern hemisphere where precipitation minus evaporation is mostly driven by evapotranspiration. Even if a random parameter is selected correlation will always be higher because the meteorological forcing is the precipitation - evaporation is seasonal. This modified KGE$_{\alpha\beta}$ ~~(Eq. ??)~~ only depends on variability (α) and bias (β) and variants of it have been used also in other studies (see, e.g., Martinez and Gupta, 2010; Mai, 2023). We utilize observed neutron count data from CRNS and estimated neutron count data from the mHM ~~model~~ to calculate various metrics such as the modified Kling-Gupta efficiency coefficient (KGE$_{\alpha\beta}$), ~~Nash-Sutcliffe efficiency (NSE)by Nash and Sutcliffe (1970), coefficient of determination (R^2) by Kvålseth (1985),~~ root mean square error (RMSE), and percentage bias (PBIAS) by Gupta et al. (1999). The optimal PBIAS value is 0, with lower values indicating more accurate model simulations. Positive values indicate underestimation by the model, while negative values indicate overestimation. This approach allows us to minimize uncertainty in the simulated neutron count data by comparing it to observed data and determining the optimal parameter values for the mHM ~~model~~. A summary of the individual parameters and their ranges can be found in Supplementary Table ~~S1 and model performance measures are shown in Table 2.~~

$$
\begin{aligned}
\text{KGE} &= 1-\sqrt{(\alpha-1)^2+(\beta-1)^2+(\rho-1)^2}\,,\\
\text{KGE}_{\alpha\beta} &= 1-\sqrt{(\alpha-1)^2+(\beta-1)^2}\,,\\
\text{with Variability } \alpha &= \sigma_{\text{sim}}/\sigma_{\text{obs}}\,,\\
\text{Bias } \beta &= \mu_{\text{sim}}/\mu_{\text{obs}}\,,\\
\text{Correlation } \rho &= \rho(\text{sim},\text{obs})\,,\\
\text{NSE} &= 1-\frac{\sum_{i=1}^{n}(y_{\text{sim,i}}-y_{\text{obs,i}})^2}{\sum_{i=1}^{n}((y_{\text{obs,i}}-\overline{y}_{\text{obs,i}})^2}\,,\\
\text{R}^2 &= \left(\frac{\sum_{i=1}^{n}(y_{\text{obs,i}}-\overline{y}_{\text{obs,i}})(y_{\text{sim,i}}-\overline{y}_{\text{sim,i}})}{\sum_{i=1}^{n}\sqrt{(y_{\text{obs,i}}-\overline{y}_{\text{obs,i}})^2}\sqrt{(y_{\text{sim,i}}-\overline{y}_{\text{sim,i}})^2}}\right)^2,\\
\text{PBIAS} &= 100[\%](1-\beta)\,.
\end{aligned}
$$

S3.

~~Performance evaluations for the daily neutron counts simulation with observed CRNS dataset.~~ ~~**Indices $\text{KGE}_{\alpha\beta}$ KGE NSE R^2 PBIAS**Range $-\infty$ to 1 $-\infty$ to 1 $-\infty$ to 1 0 to 1 $-\infty$ to ∞ Optimal Value 1 1 1 1 0 Satisfactory Value >0.70 >0.80 >0.50 >0.65 $<\pm5$~~

3 Results

3.1 Analysis of posterior parameters across the study sites

3.2 ~~Constraining of the parameter distribution N_0 / Sensitivity Analysis~~

~~The sensitivity and uncertainty analysis performed in this study use a Latin Hypercube Sampling (LHS) approach, resulting in parameter distributions that large sample size was chosen to comprehensively explore the parameter sets and capture a wide range of possible parameter combinations in the prior range. The LHS approach creates a random value between the min and max values of~~ Figure. 4 shows the normalized range of posterior parameter sets of mHM, compared across the four study sites: *Grosses Bruch*, *Hohes Holz*, *Hordorf*, and *Cunnersdorf*. Out of 30 parameters, the ~~parameter set. Initial parameter ranges and exploratory model runs are set based on literature values (Boeing et al., 2022; Kumar et al., 2013b). Supplementary Table S1 shows the values for the parameters in all 100 000 simulations and the selected 29 parameters for the Desilets method and 31 parameters for the COSMIC method, which include snow, soil moisture, and neutrons modules as behavioral simulations, with the posterior mean of the top~~ 10 ~~best parameters set. For further information and additional details about the calibrated parameters for each site, refer to Supplementary TableS2. Among the calibrated parameters , the N_0 parameters are different in each method since this parameter does not exactly have the same physical meaning in the Desilets and the COSMIC methods.~~

~~Fig~~most relevant parameters for root-zone soil moisture dynamics are presented (see Table 2 for parameter description and ranges). The other parameters are shown in the supplementary material. Figure. 4 ~~displays the x-axis in gray, representing the original parameter range (600–1500) prior distribution for the Desilets method and (100–400)for COSMIC method. Meanwhile, the colored sections in brown, green, and purple indicate the parameter values of the calibration from the posterior distribution taken from the top-performing parameter sets for each study site. The most sensitive parameters during the calibration period are $N_{0,\mathrm{Des}}$, $N_{0,\mathrm{COSMIC}}$, rootFractionCoefficient_pervious, and rootFractionCoefficient_forest of land cover classes are employed: class 1 = forest which consisted of permeable areas covered by coniferous, deciduous, and mixed forests; class 2 = impervious cover with land uses like settlements, industrial parks, roads, airport runways, and railway tracks; and class 3 = permeable cover covered by fallow lands, or those surfaces covered by crops, grass, and orchards. The calibration process notably sharpens the Probability Density Function (PDF) of these significant parameters by eliminating some of the uncertainty linked to the variance in the prior probability distributions.~~

~~For agricultural sites such as *Cunnersdorf* and *Hordorf*, the $N_{0,\mathrm{Des}}$ best estimate parameter results lie between 1000 and 1400 cph. Meanwhile, for *Hohes Holz*, the $N_{0,\mathrm{Des}}$ parameter range lies between 800 and 1000 cph, the lowest value for the calibration parameter $N_{0,\mathrm{Des}}$ is found between 800 and 900 cph due to the highest wet above biomass in the forest area. Similarly, for~~ indicates that the selected parameters showed a well-constrained distribution within their allowed range across the study sites. Among them, at the *Grosses Bruch* ~~sites, the lowest value for the calibration parameter $N_{0,\mathrm{Des}}$ is found between 800 and 900. The prior parameter distribution $N_{0,\mathrm{Des}}$ 600 and 1500 cph is the same for all four experiments.~~

~~The estimated values of $N_{0,\mathrm{Des}}$ and $N_{0,\mathrm{COSMIC}}$ obtained in our study are close to the optimal values, indicating that the model has the potential to generate accurate cosmic-ray soil moisture estimates even under dry conditions. In contrast, some hydrological models, such as HBV and PREVAH (PREecipitation Runof EVApotranspiration Hydrological response unit model; Viviroli et al. 2009), have demonstrated weaker performance in simulating soil moisture, particularly during dry conditions (Orth et al., 2015), with slightly better agreement with observations observed during wet conditions. Table **??** provides detailed information on the mean and 95% confidence interval (CI) of the parameter values of the prior and posterior simulated results of N_0. One of the important addition of this work is incorporating the lattice water account and we used the regionalization equation to calculate the lattice water which depends on the clay content with free parametersin Eqs. 2. The optimized parameter of the mHM shows the variation of the θ_{lw} ranges between (0.02–0.04)cm^{3}cm^{-3} for different sites (see Supporting Information Table S3). This behaviour and the way it was defined in Eq. 1 indicate that θ_{lw} likely represents not only soil lattice water itself, but rather the total offset of all hydrogen pools in the vicinity of the sensor (see e.g., Schrön et al., 2017; Iwema et al., 2021) .~~ site we find the most stable parameter distribution with low variability (small error bars) across most of the inferred parameters, including vertical root fractions of different vegetation types (*rotfrcoffore*, *rotfrcofperv*). A relatively higher variability (large error bars) in the posterior parameter distributions is noticed for *ptflw0*, *ptflw1* and *ptfhigdb* – these parameters are related to the estimation of lattice water and bulk density. Pedo-transfer function (PTF) related parameters that control the saturated soil water content (*ptflowconst, ptflw1, ptflw0*) at the *Hohes Holz* site showed the lowest variability, reflecting a consistent behavior for inferring these parameters at this site. The site at *Hordorf* shows moderate variability across most of the analysed parameters especially for the *orgmatperv, pfthighdb, ptflw1, ptflw0*. Overall across all the study sites, the posterior distribution of parameter *ptflowdb* exhibits high variability, reflecting the importance of further constraining of this parameter. There is a varying degree of sensitivity across the parameters, but certain parameters consistently demonstrate sensitivity across the site (*rotfrcoffore, ptflowdb, ptfhigclay, ptflowconst*). This finding aligns with previous studies (Cuntz et al., 2015; Koch et al., 2022; Demirci and Demirel, 20 , which also identified these parameters as sensitive in mHM across various study locations.

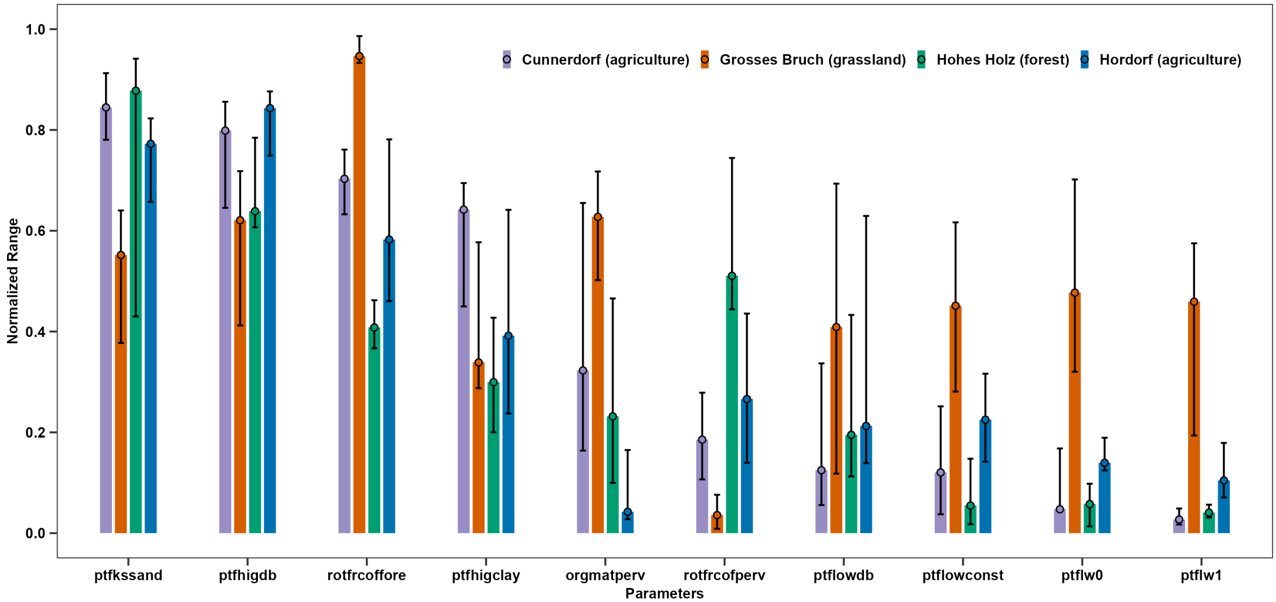

Figure 4. ~~Probability Density Function (PDF)~~ Bar plot showing posterior distribution of ~~the mHM parameter N_0 ephfor two different approaches: (a) the Desilets method~~model parameters across three land cover types, ~~and (b) the COSMIC method~~calibrated using cosmic-ray neutron sensing data. Parameter values are scaled between 0 and 1. The ~~prior PDF of~~ whiskers represent the ~~original sample, consisting~~ upper and lower limits of ~~100 000 data points, is represented by~~ the ~~grey color. The behavioral PDF~~inter-quantile range, ~~obtained after applying~~ while the ~~objective function, is shown for weighted (brown), uniform (green), and COSMIC (purple). The black dashed line represents~~ dots represent the ~~one N_0 ephvalue that best fits~~ median values of the ~~data~~normalized range for each parameter.

Table 2. ~~The four most right columns are the posterior ones~~ Description of ~~size 100 000~~ ten selected parameters and ~~are the same for all sites. The posterior distributions correspond to the distributions~~ their ranges in ~~the behavioral sample obtained after the application of the objective function~~ mHM. ~~The values correspond to the median (Q_{50}) and the lower and upper bound of the 95% confidence interval ($Q_{2.5}$ and $Q_{97.5}$, respectively).~~

Parameter No
~~$N_{0\,(\text{Des,U})}$~~ $\beta 1$
$\beta 2$
$\beta 3$
$\beta 4$
$\beta 5$
~~$N_{0\,(\text{Des, W})}$~~ $\beta 6$
$\beta 7$
$\beta 8$
$\beta 9$
$\beta 10$

~~$N_{0\,(\text{COSMIC})}$ Q_{50} 250 225234 287 316 $Q_{2.5}$ 108 202 216 265 281 $Q_{97.5}$392 249 241 302 339 mean 250 226 232 285 312 sd 87 18 9 12 19~~

3.2 Time series analysis of simulated neutron counts

The study conducts simulations of neutron counts in mHM using soil moisture parameterizations, with results presented in Figs. 5–6 across different ~~sites. The~~ land cover sites. In these figures, the grey dots represent the CRNS soil moisture measurements. The N_0 parameter values, taken from field measurement, are documented for each site, including *Grosses Bruch, Hohes Holz, Hordorf, and Cunnerdorf*. We utilized measurement data from COSMOS Europe Bogena et al. (2022), where neutron counts were converted to soil moisture, $\theta(N)$, using the methodology from Desilets et al. (2010). The simulated neutron counts were based on the simulated soil moisture content at the modeled soil horizons i.e., 0–5 cm, 5–25 cm, and 25–60 cm. The results of the ensemble runs show that the precision is higher for the behavioral simulation ensembles 0.1 %

(represented by dark gray shaded areas) than in the unconstrained simulated data 1 % (represented by light gray shaded areas). We select the best 0.1 % with the highest KGE from 100 000 model runs, and the results are presented in Tab. 3.

~~The~~ However, a larger discrepancy was noted at *Hohes Holz* a dense forest site, across all three methods. This difference could be attributed to the Leaf Area Index (LAI), biomass and vegetation dynamics, which are not currently integrated into mHM. Recent efforts by Bahrami et al. (2022) aim to address vegetation dynamics in mHM, but this integration is still incomplete. Among the methods, the N_{COSMIC} method performs best at the forest site (*Hohes Holz*), whereas at the agricultural sites (*Hordorf* and ~~Cunnerdorf~~*Cunnerdorf*), the $N_{\mathrm{Des,W}}$ method performs slightly better. ~~Only for~~ In the grassland site (*Grosses Bruch*), the uniform method $N_{\mathrm{Des,U}}$ slightly outperforms the other two methods i.e., $N_{\mathrm{Des,W}}$ and N_{COSMIC}~~, while overestimating the observations at all the other sites.~~ . In general, we observe good model performance for all methods indicated by a ~~correlation coefficient greater than 0.80~~ Kling-Gupta efficiency greater than 0.75 and a percent bias (PBIAS) below ~~2~~$\pm$ 10 % across the majority of investigated sites and methods. These results suggest that the neutron-forward models match the observed neutron counts well. However, the mean ensemble had difficulties reproducing the neutron counts for the ~~*Grosses Bruch*~~*Hohes Holz* site in all three methods.

The incorporation of dynamic vegetation in models is important as it can impact the model parameter LAI, which in turn can affect root water uptake and soil water content. Currently, these factors are not considered in the models, leading to a permanent and systematic shift in these variables each year (Zink et al., 2017; Massoud et al., 2019).

The results also highlight the uncertainties associated with model simulations and the sensitivity of the objective function. We find that ~~three~~ ten soil moisture-related parameters, ~~namely N_0, *rotfrcoffpre*, and *rotfrcofforest*,~~ mentioned in Table 2, have the most significant impact on the objective function $\mathrm{KGE}_{\alpha\beta}$, compared to the other parameters of mHM. The parameter ~~N_0~~ *lw* directly affects the neutron count simulations, while the ~~parameters *rotfrcoffpre* and *rotfrcofforest*~~ other parameters correspond to the fractions of vegetation roots in different soil layers that directly affect the water availability related stress for the estimation of actual evapotranspiration, and thereby the soil-water dynamics (Samaniego et al., 2010b; Kumar et al., 2013b). The best parameter set values in mHM across all sites and methods are given in (Supporting Information Table ~~S2~~S3).

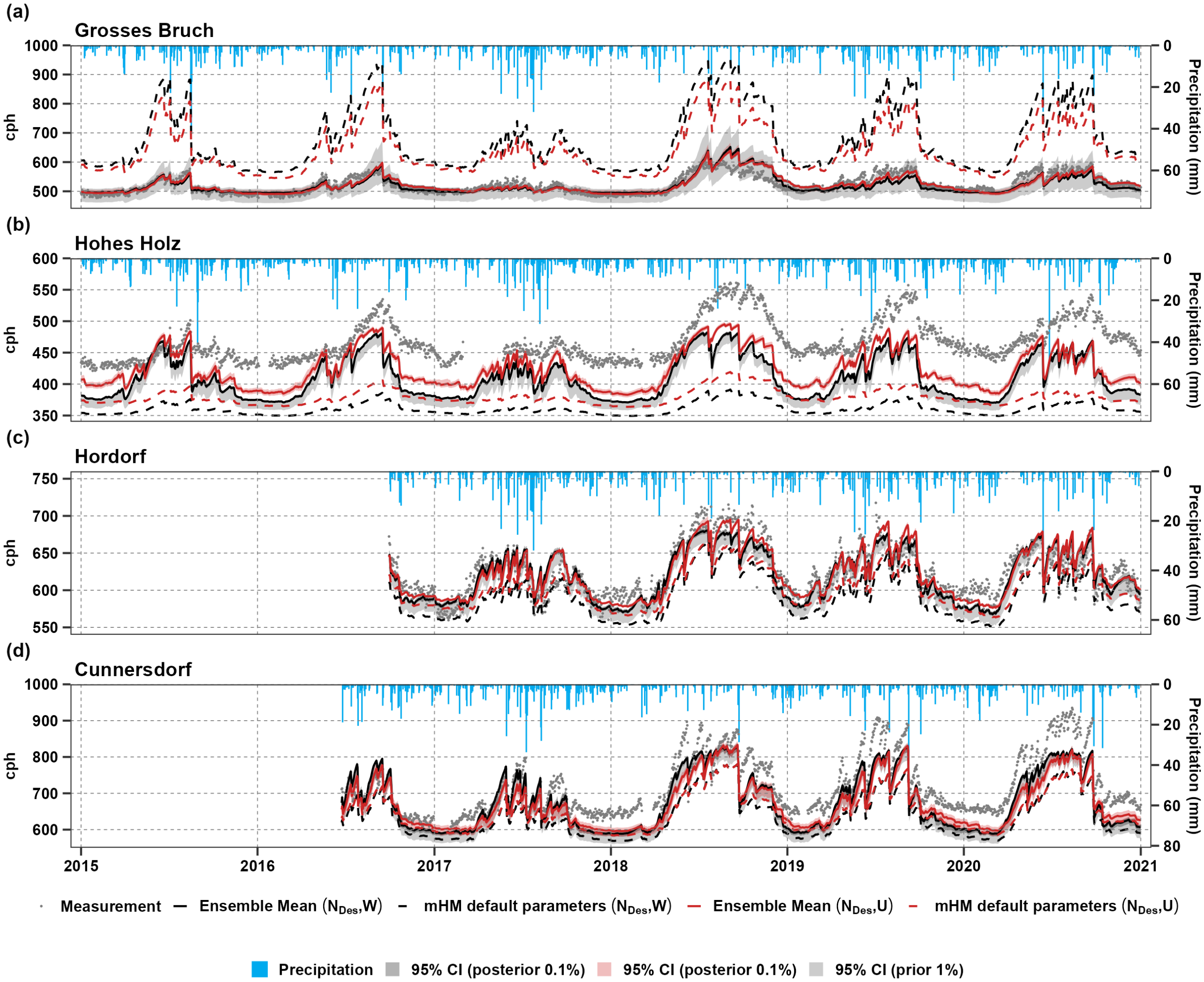

Figure 5. Simulated daily time series of black for $N_{\mathrm{Des,W}}$, red for $N_{\mathrm{Des,U}}$ for the four sites. The black lines represent the median of the behavioural simulation ensembles that satisfy the objective function which is LHS10 ensemble members. The light grey shaded areas represent the 95% CI of the simulation ensembles corresponding to different levels of constraining which is LHS1000 ensemble members, and the observation is shown in grey points. Precipitation is shown in blue color on the top.

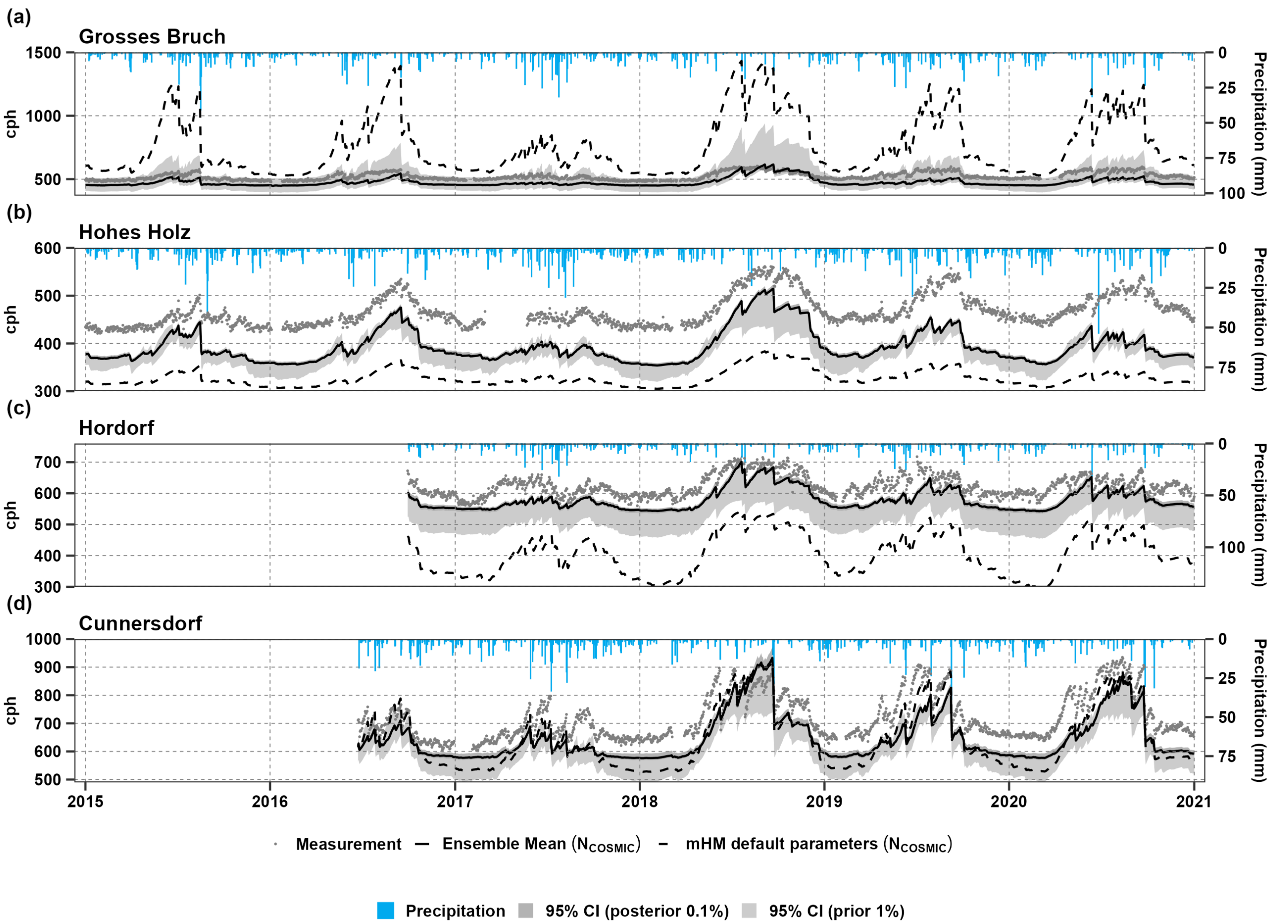

Figure 6. Simulated daily time series of N_{COSMIC} for the four sites. The black lines represent the median of the behavioural simulation ensembles that satisfy the objective function which is LHS10 ensemble members. The light grey shaded areas represent the 95% CI of the simulation ensembles corresponding to different levels of constraining which is LHS1000 ensemble members, and the observation is shown in grey points.

3.3 Model calibration statistics and evaluation

In addition to $\mathrm{KGE}_{\alpha\beta}$, the ~~four~~ three metrics KGE, ~~NSE, R,~~ RMSE, and PBIAS are used to evaluate further the mHM neutron counts simulated with observed CRNS data. We employ LHS to generate a parameter sample of 100 000 for the three methods, namely $N_{\mathrm{Des,U}}$, $N_{\mathrm{Des,W}}$ and N_{COSMIC}, by uniformly distributing the ranges provided in the (supplementary Table ~~S1~~S2). The top 10 parameter sets are found to perform satisfactorily with a KGE range of ~~0.80 to 0.93~~0.75 to 0.9, as demonstrated in Table 3. The calibrated parameter sets obtained from different objective functions are also evaluated and compared using various statistical indices, as shown in Figure 7~~, with most objective functions performing better than satisfactory based on the criteria in Table 2~~. The results for the COSMIC method indicate that the main contribution to poorer results during the evaluation period was due to the variability term (α). The boxplot displayed in Figure 7 illustrates the threshold achieved by the top 1000, 100, and 10 LHS members, along with the corresponding percentage of the best 10 LHS parameter sets that meet the threshold~~, as specified in (see Tab. 2). Among the 31~~. Among the 30 parameters selected to simulate neutron counts, this plot provides an overview of the distribution of results and their variability with respect to the threshold criteria.

Table 3. Performance metrics for model calibration (2014-2021) using various methods: ~~Percent bias~~ Kling-Gupta Efficiency (~~PBIAS~~KGE), ~~coefficient of determination~~ Root Mean Square Error (~~R^2~~ RMSE), ~~Nash-Sutcliffe efficiency (NSE),~~ and ~~Kling-Gupta Efficiency~~ percentage bias (~~KGE~~PBIAS) across different sites. ~~Bold values indicate~~ The observed neutron counts were compared with the ~~best performance measures~~simulated neutron counts from the mHM.

Sites	***Grosses Bruch***			***Hohes Holz***			***Hordorf***			***Cunnersdorf***		
Methods:	$N_{\mathrm{Des,U}}$	$N_{\mathrm{Des,W}}$	N_{COSMIC}	$N_{\mathrm{Des,U}}$	$N_{\mathrm{Des,W}}$	N_{COSMIC}	$N_{\mathrm{Des,U}}$	$N_{\mathrm{Des,W}}$	N_{COSMIC}	$N_{\mathrm{Des,U}}$	$N_{\mathrm{Des,W}}$	N_{COSMIC}
mHM default run												
KGE	-0.74	-1.46	-5.52	0.33	0.26	0.44	0.73	0.81	-0.06	0.63	0.71	0.64
RMSE	133.78	175.1	309.8	89.61	108.15	139.5	27.46	36.31	223	80.41	90.18	85.5
PBIAS	23.3%	30.2%	46%	-18.6%	-22.6%	-29.6%	-3.5%	-5.2%	-35.2%	-9.8%	-11.6%	-10%
mHM calibrated												
KGE	0.85	0.83	0.78	0.77	0.75	0.79	0.87	0.86	0.84	0.81	0.90	0.85
RMSE	16.12	17.84	50.55	45.42	59.9	73.5	16.83	17.89	48	54	51.83	81
PBIAS	0%	-0.7%	-9%	-8.7%	-12%	-15.4%	-0.1%	-0.6%	-15.4%	-6.2%	-5.7%	-9.9%

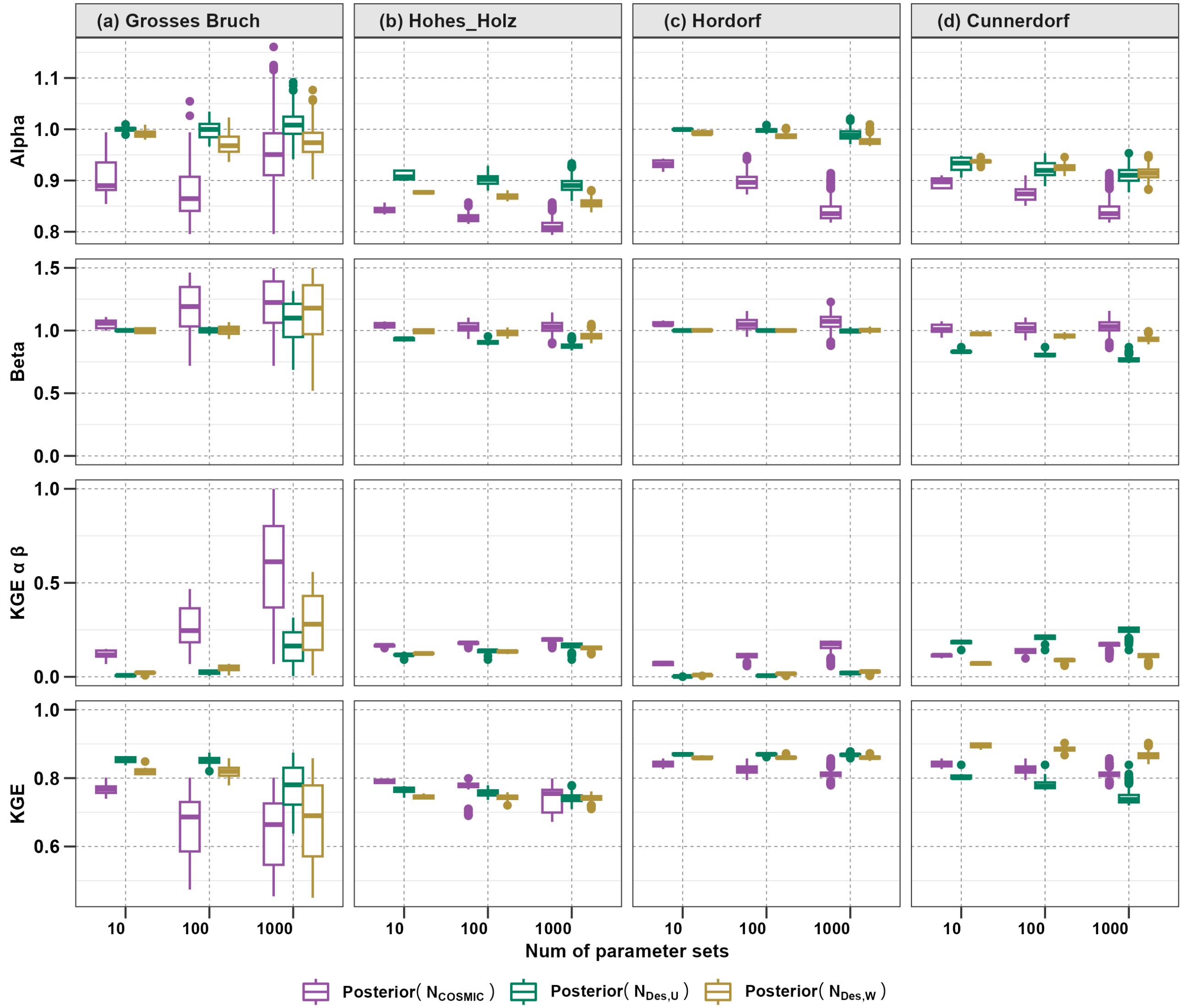

Figure 7. Evaluation of model performance using boxplots constraining of 1000 to the best 10 parameters set at four different sites, using three different methods, namely $N_{\mathrm{Des,W}}$ in brown, $N_{\mathrm{Des,U}}$ in green, and N_{COSMIC} in purple. The figure presents four subplots, where (a) represents Alpha, (b) Beta, (c) $\mathrm{KGE}_{\alpha\beta}$, and (d) Kling-Gupta efficiency (KGE) and its components, i.e., the variability term (perfect value: 1), and bias term (perfect value: 1), respectively.

3.4 Comparing evapotranspiration at Hohes-Holz: eddy covariance observed data vs mHM simulation

The ensemble model of (10 members) simulations ~~, is further examined with the~~ are further validated with evapotranspiration (ETa) ~~to cross-evaluate and~~ data to assess the model's ability to represent other fluxes and states ~~next~~ in addition to neutron counts~~by using the~~. This validation uses ETa observational data from eddy covariance measurements provided by the Integrated

Carbon Observation System (ICOS) at *Hohes Holz* ~~Warm Winter (2022)~~(Warm Winter, 2022). In terms of temporal dynamics, the model is ~~able~~ capable to capture the observed ETa quite well at the study site, as shown in Figure 8. Panel (c) displays the scatter plot incorporating linear regression models to quantify the relationships between observed and mHM-simulated ETa during both the growing and non-growing seasons. This plot provides insights into the seasonal variations in the relationship between observed and simulated ~~ET~~ETa. It suggests that the model performs best during winter, while its performance during summer is comparatively weaker. The correlation coefficients (~~r~~ r values) for each season are as follows: autumn [SON] (~~r~~ r = ~~0.79~~0.72), spring [MAM] (~~r~~ r = ~~0.77~~0.75), summer [JJA] (~~r~~ r = ~~0.42~~0.35), and winter [DJF] (~~r~~ r = ~~0.87~~0.85). It is worth noting that winter shows the highest correlation between observed and simulated ~~ET~~ETa, while summer exhibits the lowest correlation. The most significant deviation in terms of RMSE is evident during the summer, when ~~evapotranspiration~~ ETa is highest, while the smallest difference is in winter when ~~evapotranspiration~~ ETa has less impact. The model slightly overestimates ~~evapotranspiration~~ ETa in summer and spring, possibly because of the absence of a dynamic vegetation growth module in the mHM, also discussed for evapotranspiration ~~in~~ by Zink et al. (2017). The temporal dynamics of the model-simulated evapotranspiration are in good agreement with the observed data from the *Hohes Holz* forest eddy covariance site, taken from Warm Winter (2022), as illustrated in Figure 8a. ~~The daily~~ Daily correlation between observed and simulated evapotranspiration is observed high in the growing season at ~~$r = 0.84$~~$r = 0.8$, whereas the lowest correlation is found in the non-growing season at ~~$r = 0.65$~~ $r = 0.53$ in Figure 8c. The highest deviation in terms of RMSE is observed during summer when the highest fluxes occur, and the lowest during winter, in which the contribution of ETa is lowest.

In Figure 8b, the prior and posterior parameter distributions of evapotranspiration for *Hohes Holz* are displayed. The prior distribution represents the 100 000 parameters set utilized for the neutron counts simulation under Latin Hypercube Sampling (LHS). The results demonstrate that the ensemble model of 10-member simulations (posterior) for neutron counts can also effectively capture evapotranspiration, exhibiting a root mean square error (RMSE) of 0.76 mmd^{-1} of the growing season and 0.25 mmd^{-1} for non-growing when compared to observed ICOS data and simulated mHM. When compared to the model simulations with prior parameter sets, we notice a substantial improvement in ET simulations (mean RMSE of ~~0.86~~ 0.85 mmd^{-1} to 0.76 mmd^{-1}). Furthermore, the RMSE range is also narrower for the posterior simulations compared to the prior ones which further demonstrated the additional value of incorporating CRNS measurements in improving the consistency of both modeled soil moisture and evapotranspiration estimates. Nevertheless, the overall agreement between modeled and observed ETa is reasonably good; and the analysis reveals further improvement of model performance in the growing season.

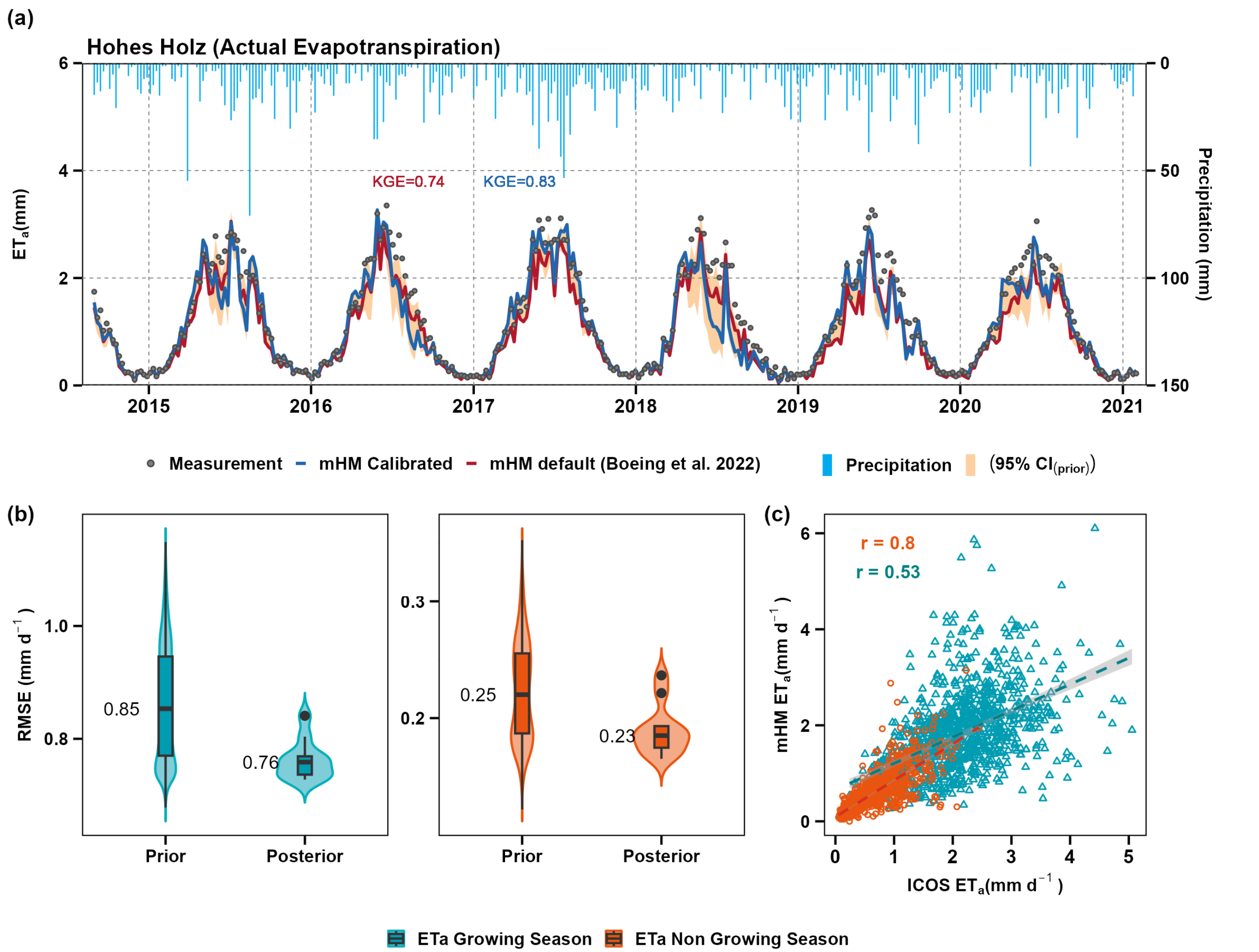

Figure 8. (a) ~~Time series~~ Comparison of weekly observed actual evapotranspiration (~~ETa~~grey dots) ~~from~~ and simulated actual evapotranspiration using the default mHM parameters by Boeing et al. (2022) (~~black~~red line), ~~ICOS measurement~~ the calibrated simulation (~~red~~blue dots), and the prior range of 100 000 realizations in (orange) color over the *Hohes Holz* site. (b) Boxplot of daily actual evapotranspiration (ETa) differences between the growing and non-growing seasons, comparing two selected prior with 100 000 simulations, the values represent the mean of the statistical metrics and posterior with 10 ensemble member distributions using the root mean square error (RMSE) as the evaluation metric (μgm^3). (c) scatterplots of modeled vs. observed ET on a daily basis from ICOS during the growing season from March to August (green) and non-growing season from September to February (brown) at *Hohes Holz* eddy covariance station in a forest.

4 Discussion

This study assessed the suitability of CRNS observations at four sites to enhance soil moisture representation in mHM. The theoretical measurement depth for the cosmic-ray probe varies, ranging from $\sim$ 12 cm in wet soils to $\sim$ 76 cm in dry soils (Zreda et al. (2008, 2012a); Rosolem et al. (2014)).

To improve the soil moisture profile representation within mHM it is a major challenge to use a single vertically integrated CRNS measurement. In order to have a fair comparison between the model and observed CRNS data, two conceptually different approaches were integrated into mHM to calculate neutron counts from different SWC horizon depths i.e., an empirical method based on Desilets et al. (2010), and ~~a physics-based method~~ neutron forward operator (COSMIC) based on Shuttleworth et al. (2013). Since the empirical method is described by an analytical expression, taking into account the uniform average of the soil moisture layers, it is straightforward to implement and therefore most commonly used (Zreda et al., 2012b; Rivera Villarreyes et al., 2011; Andreasen et al., 2017; Bogena et al., 2022). However, the method comes with the risk of missing a representation of the vertical profile of soil properties and water content. Therefore, we extended this uniform-averaging scheme with a vertical weighting scheme to mimic the sensitivity of the neutrons to the upper layers both weighted and non-weighted soil moisture approaches in the context of CRNS have been discussed (Rivera Villarreyes et al., 2014; Baroni and Oswald, 2015; Schreiner-McGraw et al., 2016; Zreda, 2016; Schrön et al., 2017; Vather et al., 2019; Barbosa et al., 2021). The COSMIC operator also accounts for the full soil moisture profile, ~~but in a more physically behaved manner,~~ following the track and attenuation of the neutrons in and out of the soil column. The mHM ~~model~~ is now able to simulate neutrons directly with all three approaches. The presented results confirmed general consistency with CRNS observations at four sites in Germany (Figs. 5 and 6).

Agricultural land presents a valuable opportunity to examine the interaction between soil moisture dynamics, crop growth, irrigation methods, and vegetation dynamics. *Hordorf* and *Cunnerdorf* are specific agricultural sites where seasonal changes in aboveground biomass are expected to be larger due to crop growth and harvest compared to grassland and forest sites. The study by Schrön et al. (2017) found that the revised weighting strategy for CRNS data improved the accuracy of soil moisture predictions at agriculture sites, but there is still room for improvement in capturing local dynamics through revised parameters in the CRNS model. Our results also showed that at the agriculture site, the ~~$N_{\mathrm{Des,W}}$~~ $N_{\mathrm{Des,U}}$ methods in mHM slightly out-performed the other methods.

We also investigated *Hohes Holz*, a forest site, and observed an early simulation of approximately 28 days in the simulation of neutron counts compared to the observations. The early simulation phase could be attributed to the limitation of mHM in simulating the dynamics of detailed vegetation mechanisms Zink et al. (2017). ~~One specific limitation is that the model does not fully account for the fact that trees at the site have access to deeper water sources, which can result in water stress being experienced at later times. Still, we get very good results in terms of KGE, for instance, indicating that these issues are of minor importance and that all three methods in mHM representation of the forest are already performing quite well.~~ While CRNS and TDR generally agree at this site, the discrepancy shown in our results could be attributed to issues related to process representation in mHM Boeing et al. (2022). Simulation of neutron data within the mHM ~~model~~ and subsequently comparing it with observed counts can enhance the accuracy and precision of soil moisture measurements. Future research can focus on exploring the potential relationships between CRNS data and soil moisture anomalies, thus furthering our understanding of the dynamics of drought and assisting in the development of efficient drought monitoring and mitigation strategies.

To cross-evaluate our results, we generated and filtered the 100 000 regionalized parameter sets based on observed neutron counts for behavioral solutions. After selecting the most effective solutions, we conduct cross-validation by comparing the mHM simulations of evapotranspiration against observational data from eddy covariance measurements ICOS (Warm Winter, 2022; Pohl et al., 2023) at the *Hohes Holz*. Figure 8 shows the scatter including the seasonal correlation coefficient at the forest site. The results indicate low correlations in summer, likely due to mHM's limitations in capturing evapotranspiration values with mHM's static vegetation module. However, the model performs well in winter, with a high correlation between observed and simulated values of evapotranspiration, the results confirm the findings from Zink et al. (2017), who used mHM to estimate evapotranspiration, groundwater recharge, soil moisture, and runoff with 4 km spatial and daily temporal resolutions (1951–2010). They utilized soil moisture observations from eddy covariance stations employing Time-Domain Reflectometer (TDR) or Frequency-Domain Reflectometer (FDR) sensors. Due to disparities in spatial representativeness and sampling depth, a direct comparison between observed and simulated soil moisture was not feasible, their findings revealed deviations in evapotranspiration during spring and in cropland areas, while soil moisture estimations exhibited good agreement with observed dynamics. The study highlights the importance of considering seasonal variations when analyzing the results. Discrepancies, such as low correlations in summer, indicate the need for improvements in capturing evapotranspiration dynamics under varying environmental conditions. Refining vegetation dynamics representation could enhance the simulation of evapotranspiration processes. Additionally, the agreement between mHM and observed soil moisture dynamics suggests variable model performance for different hydrological variables, emphasizing the need for a comprehensive assessment of its capabilities across various environmental conditions and spatiotemporal scales. The accuracy of modeled evapotranspiration is linked to soil parameterization because soil water is the main source of evaporative water. During the growing season (summer), the model exhibited the largest variability in modeled ETa (Figure 8c). This can be associated among other things with a lack of a dynamic vegetation growth module in mHM, which may not capture the onset of the vegetation period adequately. This variability could also be attributed to seasonal changes in vapor pressure difference (VPD) or more localized processes occurring at the forest site (e.g., ~~under-story vegetation~~ vegetation dynamics), which are currently not considered in the model. ~~The comparison of observed neutron counts with simulated counts from mHM improved not only soil moisture estimation but also evapotranspiration estimation in the model. This provides evidence that CRNS data has the potential to improve hydrological process understanding as a whole.~~

The *Grosses Bruch* site stands out as a mesophilic grassland site with a nearby water channel, shallow ground water, regular cattle grazing, and seasonal flooding (Hermanns et al., 2021). We find ~~a large ensemble-related uncertainty at this site for all three methods, while~~ the uniformly weighted approach $N_{\mathrm{Des,U}}$ shows a slightly better performance than the other two methods $N_{\mathrm{Des,W}}$ and N_{COSMIC} (see Table. 3). The behaviour may result in a missing representation of locally significant hydrological components, such as dynamic biomass, snow, shallow ground water, or nearby surface ponding (Schrön et al., 2017). ~~Moreover, in the middle of September, many cows had been present at this site, which could have led to a non-negligible variation of the neutron signal and thus to a non-meaningful expression of correlation-related measures Schrön et al. (2017).~~

~~Döpper et al. (2022) mentioned thigh~~ Döpper et al. (2022) mentioned high impact of grazing on the plant traits and soil properties at this site. Additionally, the use of one grid cell measurements by mHM in our study may have limited the accuracy of our results, as the depth of measurement may not be representative of the entire soil profile. Notably, neutron counts were found to provide a more accurate representation of soil water content during June, July, August, and September, when levels tend to be lower. Further exploration of neutron counts may yield additional improvements to model performance.

Overall, the three methods ($N_{\mathrm{Des,U}}$, $N_{\mathrm{Des,W}}$, and N_{COSMIC}) in mHM were able to consistently simulate the neutron count variability throughout the available data period, with the exception of the Hohes Holz site. However, a broader confidence interval is observed, indicating a greater range of variations, which implies a higher degree of uncertainty in the N_{COSMIC}. The COSMIC approach ~~explicitly accounts for water content snow~~is more complex than the Desilets approach and as such depends on more detailed additional information about the soil properties, vegetation interception, ~~and root-zone soil processes that may likely lead to a better representation of observed neutron count variation compared to Desilets that empirically represent such processes~~layering, etc. If the model input data is not known in such a detail, we would expect the COSMIC model to provide more uncertain results. Moreover, all three approaches are rough approximations of the actual physical processes of neutron transport which could contribute to systematic biases of around 2 % compared to exact physics-based models (Shuttleworth et al., 2013). The simulated time series tended to slightly underestimate the CRNS neutron count rate, particularly during the dry season. This effect could be explained by the known limitations of the equations under very dry conditions, while recent approaches exist (Köhli et al., 2021) that could lead to further improvement in future studies. Nevertheless, the results generally confirmed the slightly better performance of the weighted approach $N_{\mathrm{Des,W}}$~~than~~ , compared to the uniform $N_{\mathrm{Des,U}}$, because of its more realistic representation of neutron propagation with depth. After optimizing the soil hydraulic properties based on CRNS data, the integrated signal was reproduced very well (Fig. 5). ~~The better performance of N_{COSMIC} and $N_{\mathrm{Des,W}}$ over $N_{\mathrm{Des,U}}$ demonstrates the benefits of explicitly resolving individual soil moisture profiles, bulk densities, and lattice water, as opposed to a uniform average across the layers. This perception, however, might depend on site-specific soil profile characteristics and be less prominent if profiles are largely uniform or incorrectly resembled by the model structure. We also included offset hydrogen pools in the form of lattice water to the~~ Previous studies, such as McJannet et al. (2014) or Baatz et al. (2014), have noted low experimental performance for the Universal Calibration Function (UCF) method described by Franz et al. (2013). However, we have selected the Desilets method, known as the N_0 ~~calibration function , which was important for more accurate soil moisture estimates, confirming initial suggestions by Bogena et al. (2013). Moreover, a strong correlation between biomass and the N_0 parameter was reported in several studies (Franz et al., 2013; Hawdon et al., 2014; Baatz et al., 2014, 2015). In our study, we pass the N_0 parameter as a calibration parameter set in~~ method, and the COSMIC method for specific reasons. Both methods require information from soil profiles, which is readily available in the mHM. In contrast, the Universal Transport Solution (UTS) function couples soil moisture with air humidity in a non-separable way, while no atmospheric information about air humidity is available in the distributed hydrological model mHM. The same holds for the UCF function, which additionally requires a number of parameters related to hydrogen pools not represented by mHM. In using the CRNS soil moisture measurement the drier locations show larger deviations than the wetter locations (Iwema et al., 2015). The possibility of using simulated high-resolution soil moisture profiles instead of a few measurements at different soil depths could further increase the accuracy of the model predictions (Brunetti et al., 2019). ~~One of the primary sources of uncertainty at the *Grosses Bruch* site is surface ponding and shallow groundwater, as well as the loamy texture of the soil. Those factors contribute to the formation of permanent water ponds in the area and may introduce uniform or even inverse soil moisture profiles which directly influence the neutron emissions, but cannot be captured by the mHM model. Another factor is the time-variable effect of crowding cows near the station, which may influence the CRNS signal, but is challenging to correct in the CRNS measurement (Schrön et al., 2017). We incorporate the CRNS parameter set in mHM, and some parameters related to soil moisture and neutron counts are effectively constrained based on the objective function using KGE$_{\alpha\beta}$. However, there is still room for improvement, particularly with regard to the coefficient in root fractions distributed across soil layers.~~

~~According to Beck et al. (2021), model calibration provides more overall benefits than data assimilation. Furthermore, model calibration can be advantageous for regions with both sparse and dense rain gauge networks, whereas data assimilation is more beneficial for regions with sparse rain gauge networks. In this paper, the Latin Hypercube Sampling (LHS) method McKay and Conover (1979) is adopted to generate input variable samples, which is a stratified sampling method that reduces the number of simulations required compared to the conventional Monte Carlo method Iman and Helton (1988). LHS divides the range of each input into N intervals and selects one representative value from each interval to ensure full coverage of the input variables range and representation of all possible values in the simulation.~~ Previous studies by Smith et al. (2019) and Liu et al. (2022) address the challenges of using the original KGE in Markov chain Monte Carlo (MCMC) methods, offering insights for accurate parameter estimation and posterior distribution exploration. To address this issue, it is recommended to use adaptations to the LHS method instead of directly using the original KGE to improve the exploration of the posterior distributions. Our approach can estimate the posterior distributions of model parameters based on the objective function KGE$_{\alpha\beta}$ by taking the variance and bias.

~~This paper provides a framework to incorporate CRNS data into the mHM to assess the accuracy of soil water content on different land cover types, including agricultural land, deciduous forest, and grassland. The integration of methods from Desilets et al. (2010) and Shuttleworth et al. (2013) in mHM , using climatic data and soil physical parameters, the parameterization of evapotranspiration is effectively improved (see~~ We compared soil moisture before and after calibrating neutron counts in mHM at four sites shown in (Fig. 9). ~~Additionally, Supplementary Fig. S5 illustrates the improved representation of soil moisture for Hohes Holz. This framework lies in its ability to utilize~~ The left panel shows the mHM's default simulation using the default parameter set from Boeing et al. (2022), whereas the right panel shows the calibrated simulation based on $N_{\mathrm{Des,U}}$ method. The presented depicts the CRNS soil moisture measurements (grey dots) versus the soil moisture derived from mHM in different depths (colors). Table 4 shows the corresponding performance measures. It is important to acknowledge that the optimization on observed neutron counts ~~data, allowing for a comprehensive assessment of the model's performance and enhancing its reliability in hydrological modeling~~not only improved the soil moisture representation in mHM. At the same time, it also improved the simulated evapotranspiration, as shown in the example of Hohes Holz (compare Fig. 8a). The KGE value between modeled and measured ETa by eddy covariance observations improved significantly from 0.74 to 0.83. This provides evidence that CRNS data has the potential to improve hydrological process understanding as a whole.

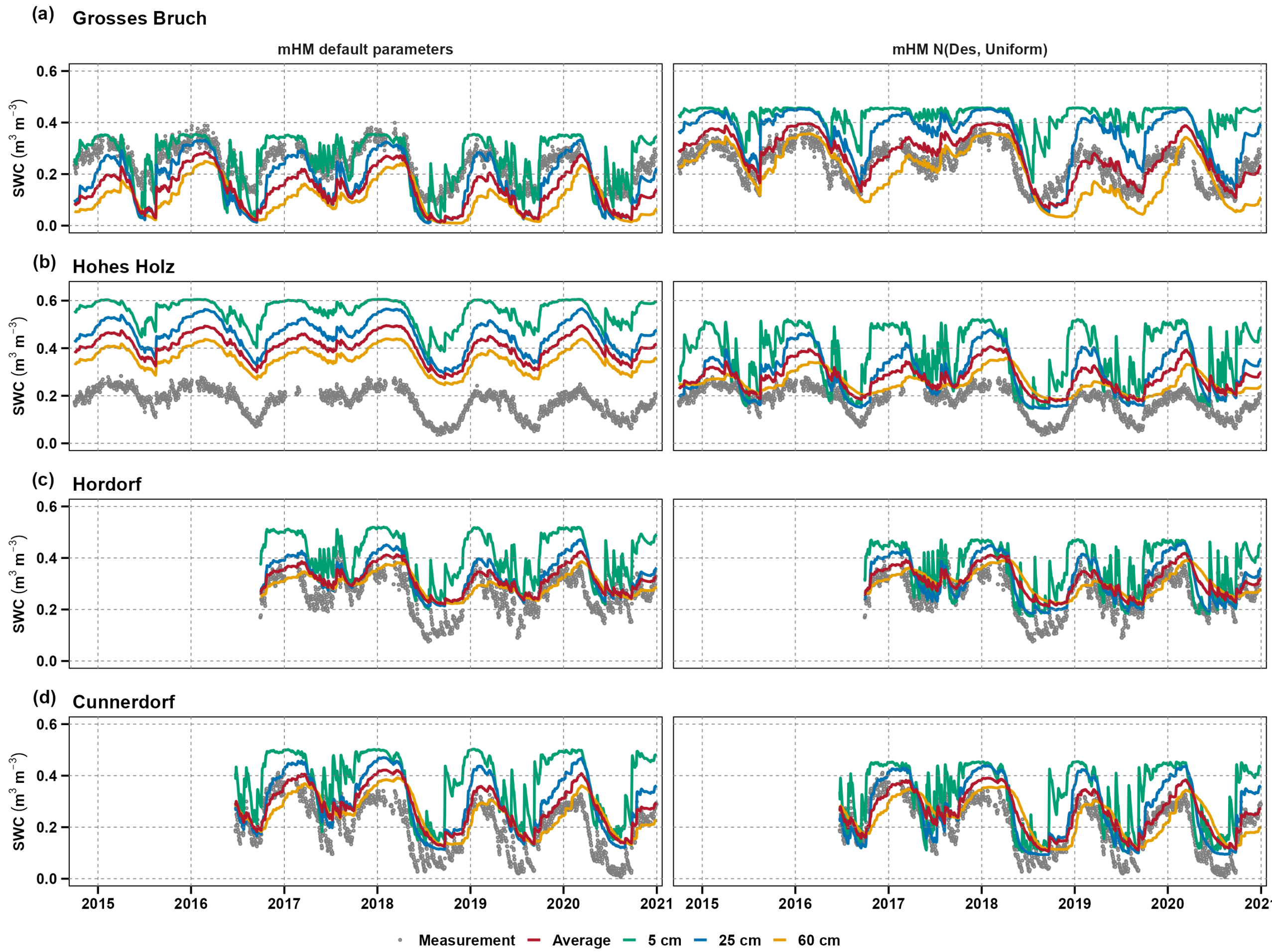

Figure 9. Comparison of ~~weekly observed actual evapotranspiration~~ soil water content (~~grey dots~~SWC) ~~and simulated actual evapotranspiration using~~ time series from (2015 - 2021) across all sites. The left panel illustrates the default simulation from mHM using parameters ~~by~~ from Boeing et al. (2022)~~(red line) and~~, while the right panel presents the calibrated simulation based on the $N_{\mathrm{Des,U}}$ method. Both panels compare CRNS-derived soil moisture data (~~blue~~ grey dots) ~~over~~ with simulated values from mHM. The best 10 calibrated mean SWC values across different soil layers are shown, with the ~~*Hohes Holz* site~~total average soil moisture represented by the red line.

Table 4. Performance metrics (KGE, RMSE, and PBIAS) for soil moisture simulations across four sites from (2014 - 2021) between θ_{CRNS} against simulated data from mHM : *Grosses Bruch, Hohes Holz, Hordorf, and Cunnersdorf*. The results are compared between the default mHM run and three calibration methods ($N_{\mathrm{Des,U}}$, $N_{\mathrm{Des,W}}$, and N_{COSMIC}).

Sites	*Grosses Bruch*				*Hohes Holz*				*Hordorf*				*Cunnersdorf*			
Methods:	Default run	$N_{\mathrm{Des,U}}$	$N_{\mathrm{Des,W}}$	N_{COSMIC}	Default run	$N_{\mathrm{Des,U}}$	$N_{\mathrm{Des,W}}$	N_{COSMIC}	Default run	$N_{\mathrm{Des,U}}$	$N_{\mathrm{Des,W}}$	N_{COSMIC}	Default run	$N_{\mathrm{Des,U}}$	$N_{\mathrm{Des,W}}$	N_{COSMIC}
KGE	0.53	0.66	0.74	0.65	-0.32	0.42	0.09	0.18	0.55	0.59	0.47	0.47	0.55	0.64	0.48	0.43
RMSE	0.11	0.06	0.05	0.08	0.23	0.1	0.23	0.14	0.07	0.07	0.1	0.1	0.09	0.08	0.09	0.11
PBIAS	-44.3%	14.6%	11.5%	26.9%	131%	55%	90%	80.9%	22.4%	19%	33.8%	35%	37.6%	26.2%	39.4%	49.3%

5 Conclusion and future outlook

This study evaluates the potential of ~~the mHM a large-scale hydrological model for simulating neutron counts~~ cosmic-ray neutron observations to improve soil moisture and model parameters in the mesoscale hydrological model mHM at the 1.2 km×1.2 km scale across different land cover sites for the period 2014–2021. ~~Two empirical and one physical model approaches are evaluated for deriving neutrons from the soil moisture profile. Neutron measurement data~~ For this, we derived the neutron counts from simulated soil moisture profiles directly in the model using three different approaches: two based on an empirical function with uniform and non-uniform weighting of soil horizons, and one more complex approach based on the neutron forward operator COSMIC. Then, observed neutron counts from four sites in Germany ~~are integrated, and the influence on hydrological model parameters, as well as simulated soil moisture and evapotranspiration are analyzed. The parameter sample~~ were used to calibrate the mHM parameters. Based on the $\mathrm{KGE}_{\alpha\beta}$ between simulated and observed neutrons, the best 1 % parameter sets out of 100 000 ~~realizations for neutron counts was taken, which are analyzed regarding their uncertainty caused by the parameter estimation. The parameter sets are filtered based on the KGE of observed vs simulated neutron counts. The best 1% member ensemble simulations are evaluated with neutron counts, evapotranspiration, and soil moistureobservations~~model realizations were used to investigate the impact on the posterior parameter distribution and on the simulated neutrons, soil moisture, and evapotranspiration.

The evaluation of neutron counts ~~at four different sitesyields a KGE value of > 0.8~~yielded KGE values > 0.75 at all four sites, indicating a satisfactory representation of the neutron ~~observations. The~~ counts in the model compared to the observations for the best 1 % ensemble parameter ~~set is found more representative of 100 000 realizations, suggesting a reliable model performance~~sets. The performance of the neutron counting methods ~~varies~~ varied across different land cover types. The non-uniform $N_{\mathrm{Des,W}}$ method generally ~~demonstrates~~ showed good performance, particularly at the agricultural sites. While the N_{COSMIC} method performs slightly better at ~~forest site and the~~ the forest site. The uniform $N_{\mathrm{Des,U}}$ method ~~shows~~ showed slightly better results at the grassland site.

~~However, there~~ There is still room for improvement in ~~some areas. Specifically, working with grassland sites presented challenges, particularly with the N_{COSMIC}~~ the model representation of complex sites, e.g. to better address the special site-specific conditions of the forest or grassland site, especially when using the COSMIC method. On the one hand, it is a ~~physics-based approach incorporating a comprehensive representation of the neutron counting process~~method that aims at mimicing the physical processes of neutron transport in the soil in detailed way, but on the other hand, it relies on the detailed representation of the site characteristics in the hydrological model. This complexity could introduce additional uncertainties and limitations in the model, potentially affecting its performance, especially when the actual site is more complex than it has been modeled. The study suggests that the observed discrepancies between model and observations may be attributed to the representation of dynamic biomass, snow, surface ponding, and shallow groundwater dynamics, which are present at the grassland site, for instance. Addressing these features could further enhance the model's accuracy.

The calibration on neutron counts not only improved the soil moisture estimation but also improved the simulation of evapotranspiration at the *Hohes Holz* station. The evaluation with evapotranspiration data from eddy covariance ~~at *Hohes Holz* stations indicates~~ observations indicated some deficiencies in mHM to deal with forest systems, but also great potential for CRNS measurements to improve the water partitioning in the model as a whole. ~~Especially in~~ In the growing season (March-August), deviations of the modeled and observed ETa indicate room for better representation of mixed soils and dynamic vegetation modules at the local scale within mHM. ~~The calibration on neutron counts not only improved the soil moisture performance of the model but also helped to set the modeled evapotranspiration straight.~~

In conclusion, the incorporation of neutron counts estimation into mHM by accounting for vertical soil moisture profiles improves the model's accuracy and provides a more realistic representation of soil moisture dynamics at all four study sites and ~~evapotranspiration at~~ even evapotranspiration at the *Hohes Holz* site. This research presents a direction for future studies to explore. ~~The next step in this research is to evaluate the ability of this CRNS module in mHM for estimating soil moisture through~~ Next steps could be the evaluation of neutrons and soil moisture in mHM by a large-scale soil moisture monitoring initiative, e.g. by utilizing more stationary CRNS networks ~~or the novel rail-based CRNS data from Altdorff et al. (2023). To optimize accuracy and understanding~~(e.g., Heistermann et al., 2021; Bogena et al., 2022) or large-scale mobile CRNS campaigns (McJannet et al., 2017; Altdorff et al., 2023). To futher increase accuracy and general understanding of hydrological processes, we recommend integrating both CRNS and satellite remote sensing data into mHM (e.g., based on recent insights from Schmidt
. Improving the model predictions will contribute to reducing the uncertainties associated with drought and flood management strategies and informed agricultural decisions.

Code availability. Simulation data is attached as supplemental material. The mesoscale Hydrological Model mHM (version 5.12) is open-source and can be freely accessed from GitLab: https://git.ufz.de/mhm/mhm/-/tree/v5.12.0?ref_type=tags.

Data availability. We kindly acknowledge the German Weather Service (DWD) for providing the meteorological datasets. The terrain elevation data was collected from USGS EROS Archive - Digital Elevation - Global Multi-resolution Terrain Elevation Data 2010 (GMTED2010), available at https://www.usgs.gov/centers/eros/science/usgs-eros-archive-digital-elevation-global-multi-resolution-terrain-elevation. Gridded soil characteristics are based on the BUEK200 database obtained from the German Federal Institute for Geosciences and Natural Resources (BGR, see online at https://geoportal.bgr.de/mapapps/resources/apps/geoportal/index.html?lang=en#/datasets/portal/154997F4-3C14-4A53-B217-8A7C7509E05F). The geological dataset was downloaded from Institute for Biogeochemistry and Marine

Chemistry, KlimaCampus, Universitt Hamburg (https://www.geo.uni-hamburg.de/en/geologie/forschung/aquatische-geochemie/glim.html). Leaf Area Index (LAI) dataset was downloaded from the Global Land Cover Facility (GLCF), available at http://iridl.ldeo.columbia.edu/SOURCES/.UMD/.GLCF/.GIMMS/.NDVIg/.global/index.html. The land cover dataset was downloaded from the European Space Agency (ESA), available at http://due.esrin.esa.int/page_globcover.php. The ET data were obtained from https://zenodo.org/record/7561854.

Competing interests. RK and LS are members of the editorial board of Hydrology and Earth System Sciences.

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