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Title page

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Combining static and portable Cosmic Ray Neutron Sensor data to assess catchment scale heterogeneity in soil water storage and their integrated role in catchment runoff response

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Abstract

Soil water content (SWC) is a key variable in many land surface processes, such as runoff generation, thus knowledge about its spatiotemporal dynamics at the catchment scale can be useful for constraining and evaluating hydrological models. Cosmic ray neutron sensor (CRNS) technology provides hectare scale SWC data, and with recent advances in mobile CRNS such information value can be extended to the catchment scale, although challenges in calibration remain, especially in wet environments. This study presents a new methodology suited for humid environments to explore spatio-temporal variability in near-surface soil water storage (SNS) dynamics at the catchment scale and its value in semi-distributed rainfall-runoff modelling calibration. For a humid mixed-agricultural catchment (~10km²) in Scotland, we combined ~4-years of SWC data from a static CRNS at a landscape-representative location with “snapshots” at four key soil-land use (SLU) units to produce SWC timeseries for each one of those units. The SLU units involved a mixture of
freely draining mineral and poorly draining organic-rich soils, supporting crop and livestock farming and moorland, respectively. We also explored the suitability of the standard CRNS calibration approach in the SLU units and found that the organic-rich soils required an adapted parameter calibration for SWC. The moorland SLU unit had the greatest difference in SWC dynamics from the other agricultural SLU units. To explore the additional information generated by the combined CRNS approach, we calibrated a semi-distributed rainfall-runoff model (HBV-light) by using $S_{NS}$ dynamics in individual SLU units in addition to streamflow. Compared to a lumped approach, the semi-distributed SWC information and model structure helped produce better constrained stream flows and further improved the representation of catchment internal storage dynamics. Ultimately, the value of the SWC time series for different SLU units in rainfall-runoff modelling will depend on model structure and the degree to which $S_{NS}$ dynamics vary within the landscape. This study showed the potential of expanding the information value of permanently installed CRNS sensors using portable CRNS surveys while addressing the various challenges related to organic-rich soils and wetter environments, although testing in different environments would be required to evaluate the wider applicability.

**Key words:**

Cosmic ray neutron sensor; soil moisture; spatial variability; portable CRNS; organic-rich soils; managed landscapes; semi-distributed rainfall-runoff modelling

**1. Introduction**

Near-surface soil water storage has a key role in regulating evapotranspiration, infiltration, water retention, drainage and hence catchment runoff generation (Brocca et al., 2010; Lilly et al., 2012; Ochsner et al., 2019; Rinderer & Seibert, 2012; Tetzlaff et al., 2007). Due to its importance in many land surface processes, it is a key variable in hydrology, meteorology and agriculture (Vanderlinden et al., 2012; Vereecken et al., 2014; Western et al., 2004), and
crucial for improving land surface modelling e.g. to aid model validation and reduce the bias in prediction of water and energy fluxes (Marsh et al., 2020; McJannet et al., 2017). As such, near-surface soil water storage ($S_{NS}$), or soil water content (SWC, see Appendix I for all abbreviations) in the upper portions of the soil, is estimated by an increasing number of satellite and other observational approaches (Mccabe et al., 2017).

Cosmic ray neutron sensor (CRNS) technology can now provide field average (up to ~7 ha, Schrön et al., 2017) estimates of SWC dynamics at an intermediate scale, addressing difficulties of point scale heterogeneity and the relatively coarse spatial resolution of satellite-derived products (Fersch et al., 2018; Montzka et al., 2017; Sigouin et al., 2016). National-level networks are increasingly being installed to explore variations between sites, e.g. in USA (Zreda et al., 2012), Australia (Hawdon et al., 2014), India (Montzka et al., 2017) and the UK (Cooper et al., 2020). CRNS data have been used for a wide range of applications, including estimation of hydraulic properties (Brunetti et al., 2019; Foolad et al., 2017; Rivera Villarreyes et al., 2014), validating satellite SWC estimates (Duygu & Akyürek, 2019; Kędzior & Zawadzki, 2016; Montzka et al., 2017) and improving land surface (Baatz et al., 2017; Iwema et al., 2017) and catchment-scale environmental modelling (Dimitrova-Petrova et al., 2020a).

While CRNS probes are customarily employed at a static location providing time series of near-surface soil water contents (SWC) (Bogena et al., 2018; Coopersmith et al., 2014; Nguyen et al., 2017; Schreiner-McGraw et al., 2016), mobile CRNS technology, which includes both rover and portable CRNS applications, has the potential to expand their information value. Despite its relatively large spatial coverage, static CRNS probes are unlikely to capture fully the spatial heterogeneity in near-surface SWC of catchment (>1km$^2$) or larger scales, where higher level decision making on water resource management is generally made. In recent studies, this has been partially addressed by employing rover CRNS technology, i.e. a CRNS sensor mounted on a vehicle, providing “snapshot” maps of
spatially variable SWC across fields or within catchments. For the small catchment scale (~10 km²), spatial variability of SWC can be more easily assessed using a portable, i.e. suitcase or backpack version of the CRNS technology (Franz, 2018). Rover CRNS applications include improvement and validation of remote sensing soil moisture products at the regional scale (Chrisman & Zreda, 2013; Dong et al., 2014; McJannet et al., 2017), monitoring and soil mapping of irrigated agriculture (Finkenbiner et al., 2019; Franz et al., 2015; Gibson & Franz, 2018) and SWC characterisation in landscapes with spatially varying land uses (Vather et al., 2019). However, while the rover CRNS approach in these studies provided relatively large spatial coverage and high resolution, it lacked high temporal resolution. Alternatively, dense networks of static CRNS have been installed temporarily to investigate SWC spatiotemporal heterogeneity (Fersch et al., 2020), yet such dense monitoring systems are expensive to establish and maintain in the long term.

Therefore, an experimental framework which combines static CRNS and portable CRNS approaches has the potential to generate valuable SWC information at both relevant spatial- and temporal resolutions (Fersch, 2020; Franz et al., 2015; McJannet et al., 2017). Such an approach could be supported by the fact that at many locations under the same climatic forcing, soil moisture among sites tend to display similar dynamics at daily timescales, although with differences in magnitude. These similarities have been observed at many sites despite marked differences in land use (Choi et al., 2007; Zucco et al., 2014), hillslope position (Penna et al., 2013) or between measurements obtained at different spatial scale but at an overlapping location (Zhou et al., 2007) and soil properties (Gwak & Kim, 2017; Shi et al., 2015). However, studies that have combined static and mobile (in this case rover) CRNS approaches are limited and have mainly been tested in dry climates over large (>100 km²) areas (Franz et al., 2015) and McJannet et al., 2017)) with only a few examples in temperate sites (Jakobi et al., 2020; Schrön et al., 2018) and none in humid climates.
One challenge is the CRNS sensor calibration requirements for spatially different conditions (e.g. in soil properties or land cover). While the typical calibration of CRNS sensors works well for many sites and soil types (Bogena et al., 2013; Desilets et al., 2010), an additional evaluation of the signal correction or the sensor calibration method might be needed to address certain site-specific conditions (Heidbuchel et al., 2016; Iwema et al., 2015; Rivera Villarreyes et al., 2011). This may be in environments where high organic matter content (e.g. soil organic carbon or plant biomass) dynamically influences the signal (Bogena et al., 2013; Jakobi et al., 2018).

Indeed, in humid environments, where peaty (organic-rich) soils are often present, obtaining accurate SWC estimates remains a challenge (Boorman et al., 2018), due to the distinct water retention characteristics of these soils (Boelter, 1968). Therefore, to successfully apply combined CRNS approaches in wetter regions, testing whether an additional or flexible site-specific calibration of the neutron to soil water content (N-SWC) relationship might be a necessary pre-requisite for creating spatially variable timeseries of $S_{NS}$.

In northern, humid, mixed-agricultural catchments, near-surface SWC is a key control on runoff generation and runoff threshold response (Brauer et al., 2013; Geris et al., 2015; Seibert et al., 2011). In the UK, soil saturation and flood events are frequent so that accurate and spatially representative SWC data obtained from CRNS data could particularly help improve flood predictions (Bell et al., 2009; Hannaford, 2015; Hundecha et al., 2020). Such landscapes typically involve a patchwork of relatively small fields with variations in soil and land use/management and some proportion of wet, poorly draining moorlands on organic-rich soils (House et al., 2010). Moorlands commonly cover the headwaters of UK catchments and are known to generate large proportions of the runoff that contributes to flooding events (O’Connell et al., 2004). Thus the combination of a representative static CRNS data (Dimitrova-Petrova et al., 2020a) complemented with portable surveys within distinct soil-land use (SLU) units including more moorlands, could provide an integrated approach to
obtain spatially relevant $S_{NS}$ data in typical UK and managed landscapes. The usefulness of such spatially variable $S_{NS}$ information in hydrological modelling should be explored in each context to understand if it carries an additional value as compared to $S_{NS}$ data from a static CRNS location. In addition to hydrological modelling (Percy et al., 2020), there are many other applications which would benefit from having such spatially variable (i.e. across fields or between sub-catchments), high temporal resolution timeseries data, such as improving the efficiency of irrigation schemes (Guo et al., 2020) or evaluating the impact of land management on soil loss (Hallett et al., 2016; Vaezi et al., 2017).

The main aim of this study was therefore to use a combination of static CRNS data and portable CRNS surveys complemented with field-based SWC measurements to explore the spatio-temporal variability in near-surface soil water storage $S_{NS}$ dynamics at the catchment scale in a semi-distributed rainfall-runoff modelling framework. We applied this to a humid mixed-agricultural catchment with a range of soil-land use units including mineral and organic soils typical for the UK. More specifically, the objectives were to (i) explore the relationship between neutron intensities sensed within a landscape-representative footprint using static CRNS and those within individual/contrasting soil-land use (SLU) units using portable CRNS; (ii) based on those relationships, develop a methodology to create synthetic timeseries of daily near-surface SWC for individual SLU units addressing the challenges related to wet organic-rich soils and (iii) derive timeseries of $S_{NS}$ for the individual SLU units and demonstrate their value in semi-distributed catchment scale rainfall-runoff model calibration.

2. Methods
2.1. Site description and instrumentation

The study was conducted in the Elsick catchment (~10 km²), NE Scotland, UK (Figure 1). Mean annual precipitation is ~800 mm and potential evapotranspiration ~350 mm (Met Office, 2019a, 2019b). The underlying geology is metamorphic bedrock, overlain by glacial drift, covered by relatively thin (0-1m) soils (British Geological Survey, 2019; Soil Survey of Scotland Staff, 1981). The stream network drains a gently sloping landscape (90 to 165 m.a.s.l.) mainly covered by a patchwork of pastoral and arable farms. In this predominantly agricultural landscape, soil properties and land use are linked, forming characteristic soil-land use (SLU) units. In Elsick there are four SLU units that cover ~94% of the catchment and which are characterised by their soil drainage type (Soil Survey of Scotland Staff, 1981) and dominant land use (Table 1, Figure 1). These SLU units are: (i) Crop-Imperfectly drained (CropI), (ii) Crop-Poorly drained (CropP), (iii) Pastures-Freely drained (PastureF) and (iv) Moorland-Poorly drained (MoorlandP). Historically, the poorly and imperfectly drained SLU units associated with agriculture have been artificially drained to enhance crop growth (Blann et al., 2009; Lilly et al., 2012). The less managed, poorly drained MoorlandP sites are located in the catchment’s NE headwaters and characterised by an organic-rich surface layer (>40 cm thick). The absence of agriculture and artificial drainage makes surface ponding most frequent in this unit. A minor proportion of the catchment (~6%) has forest plantations on various mineral soils and very minor urban cover (Figure 1).

A static Cosmic neutron ray sensor CRNS_{static} (CRNS ~1000/B, Hydroinnova, New Mexico, USA) was used to obtain continuous estimates of near-surface average SWC (SWC_{static}). The CRNS_{static} station (Fig. 1C) was installed in November 2015 at the intersection of three fields (latitude 57°02′25.58″N and longitude 2°11′18.84″W, elevation = 95 m.a.s.l.), which are representative of two of the key SLU in the catchment (Table 1): CropP (Figure 1 E) and PastureF (Fig. 1 D). The CRNS_{static} sensor was calibrated over five field sampling campaigns covering a range of wetness conditions (for full details on the sensor calibration refer to
Dimitrova-Petrova et al., 2020a). The CRNS_{static} continuously records neutron intensity (N_{raw}), temperature (T), relative humidity (RH) and atmospheric pressure (P_{atm}) and, since April 2017, has been complemented by an automatic weather station (Environmental Measurements Ltd.), which measures net radiation (Kipp and Zonen NR Lite2 Net Radiometer), wind speed and direction (WSD1, Environmental Measurements Ltd.) (every 30 minutes), used alongside RH, T and P_{atm} for potential evapotranspiration estimates using the Penman-Monteith method. Precipitation was measured at the CRNS_{static} location using a tipping bucket rain gauge (EML, ARG100 gauge). Stream discharge at the Elsick catchment outlet (Q_{OUT}, in mm day^{-1}) was calculated as the sum of observations at the MAIN and TRIB sub-catchments (Figure 1 A). Gauging across the range of observed levels was used to obtain continuous stream discharge from the stream level data (TD Diver, Van Essen Instruments). Daily precipitation data prior to monitoring (January 2011 – January 2015), were obtained from distance-weighted interpolation using 14 neighbouring gauges from a national monitoring network (Met Office, 2019a) within a 35 km radius of the catchment. This was also used to fill occasional data gaps in precipitation, while site-corrected meteorological data from Dyce Aberdeen Airport (<25km to the north) were used to fill gaps in PET estimates (Met Office, 2019b).

### 2.2. Portable CRNS data collection and cross-calibration of the CRNS sensors

We combined data from the CRNS_{static} and a portable version (CRNS_{portable}) to assess the SWC in the four key SLU units situated outside (Figure 1 A) or within (Figure 1 B) the CRNS_{static} footprint. The CRNS_{portable} is similar to the backpack format described by Franz (2018). It is relatively lightweight and makes spatial surveying time and cost effective, which is well-suited for the heterogeneous landscapes with relatively small fields (Franz, 2018). These portable CRNS sensors, in contrast to the rovers, are less powerful than the static
sensors (~60% in this case), so that a cross-calibration between the two devices is required. Here, the CRNS_{portable} sensor was cross-calibrated with the CRNS_{static} sensor by deploying the CRNS_{portable} for ~8 hours next to the CRNS_{static} (Figure 1 C) on five occasions spanning a range of soil moisture conditions. The neutron counts of each sensor were integrated to 1-hour values (N_{raw} in cph). Following standard procedures, three correction factors were applied (Equation 1 and Equation 2) to account for the influence of atmospheric pressure (fp), incoming solar radiation (fi) and relative humidity (fh) (Evans et al., 2016; Zreda et al., 2012) using the data of P_{atm} (in mbar), RH, (in %) and T, (°C) recorded by each of the CRNS sensors and using a common solar intensity factor, fi (from the Jungfraujoch monitoring station, Switzerland, provided by Hydroinnova via http://nearfld.com). The signal of the CRNS_{static} was additionally corrected for the influence of aboveground biomass using a daily f_{veg} factor (following Baatz et al., (2015)) to produce daily time series of N_{pih,static}.

\[ N_{pih,static}[cph] = N_{raw,static} \times f_{p,static} \times f_i \times f_{h,static} \times f_{veg,static} \]  \hspace{1cm} (Eq. 1)

\[ N_{pih, portable}[cph] = N_{raw, portable} \times f_{p, portable} \times f_i \times f_{h, portable} \]  \hspace{1cm} (Eq. 2)

To account for the poorer potency of CRNS_{portable}, the ratio (mean ± stdev) of N_{pih, portable}/N_{pih,static} was calculated for different integration times, where we found the ratio to be stable from >4 hours. This ratio at a 4-hour integration time was then used to upscale N_{pih, portable} measured at other locations (i.e. within the individual SLU units) to N_{s, portable} (Equation 3) to enable comparable calculations:

\[ N_{s, portable}[cph] = \frac{N_{pih, portable}}{ratio} \]  \hspace{1cm} (Eq. 3)

Next, the CRNS_{portable} sensor was deployed for 8 hrs at each SLU unit (Figure 1) on 3-5 different days, covering a range of wetness conditions. We found that a linear relationship described the correlation between N_{pih,static} and N_{s, portable} for each SLU unit, as found in other studies in soil moisture spatial heterogeneity (e.g. Lv et al., 2016, Zucco et al., 2014).
The strength of these relationships (as $R^2$ for linear regression) was tested at integration times from 1 to 8 hours. As $R^2 > 0.5$ for the four SLU units was reached again at a 4-hour integration time, we used the regression at 4-hour integration time to derive continuous timeseries of $N_{\text{SLU}}$ for each SLU unit for the period 13 November 2015 - 31 December 2019 (Equation 4).

$$N_{\text{SLU}}(t) = a \times N_{\text{phv,static}}(t) + b \quad \text{(Eq. 4)}$$

Note that no vegetation correction was applied at the individual SLU units as long-term aboveground estimates were lacking for the CropI and MoorlandP units. To test the potential implications of this, we explored the differences between the relationships (Equation 4) using either vegetation corrected and non-corrected CRNSPortable data for the CropP and PastureF using t-tests. As no significant differences were found, we used time series of $N_{\text{phv,static}}$ and $N_{\text{Portable}}$ to derive the synthetic time series for each SLU unit.

2.3. Synthetic soil water content timeseries for each SLU unit ($SWC_{\text{SLU}}$)

To obtain synthetic timeseries of SWC from $N_{\text{SLU}}$ data for each SLU units (i.e. objective (ii)), we complemented the CRNSPortable surveys with independent field measurements of SWC on the same days. These were spatially distributed point SWC ($\theta$ probe) measurements and topsoil core samples (0-5 cm). For point measurements, we used a ML2 soil moisture sensor (Delta T Devices Ltd) $\theta$ probe, integrating over 0-6 cm with an approximate control volume of 30 cm$^3$. We focussed on the topsoil only as it exhibits most dynamic SWC behaviour and has been shown to strongly influence runoff generation in many agricultural sites in the UK (Gruszowski et al., 2003; Meyles et al., 2003; Withers et al., 2007). On average 140 SWC measurements in each SLU unit, on each sampling day, were made along four, 0-70 m transects radiating from the CRNSPortable location, at 90° to each other. Occasionally, technical difficulties or frozen ground limited the number of measurements possible. Usually, a minimum of two replicates were taken every 2 meters.
from 0 to 25 m distance, every 5 meters from 25 to 40 m and every 10 m from 40 to 70 m. The measurements taken with the θ probe on each sampling day (θ_{SLU}) were weighted following Schrön et al., (2017) to obtain the average soil moisture estimate for each SLU on each day.

The 0-5 cm depth soil cores were used to determine mean dry bulk density (ρ_{dry}, in [g cm^{-3}]), soil organic matter (SOM, in [cm^3 cm^{-3}]) and lattice water (LW, i.e. the water contained in soil minerals, in [cm^3 cm^{-3}]) for each SLU unit. The ρ_{dry} was determined by oven-drying each sample (24h/105°C) and correcting for stones (Hall et al., 1977), and SOM and LW estimated by loss-on-ignition (firstly 24h/450°C for SOM and then 6h/1000°C, for LW) (Davies, 1974).

The ρ_{dry}, SOM and LW for the CropP and PastureF units within the static footprint were characterised from the 0-5 cm samples from five campaigns also used to calibrate the static CRNS (Dimitrova-Petrova et al., 2020a) (n=48 for CropP and n=26 for PastureF, respectively). The ρ_{dry}, SOM and LW of the SLU units outside the footprint, i.e. CropI and MoorlandP, were characterised from a single soil sampling campaign (n=9 for the CropI and n=6 for the MoorlandP, respectively). While the sampling size for these estimates is relatively small, this is justified by the relatively low spatial variability revealed from the ~140 topsoil point SWC measurements on each sampling day in each SLU unit, and again by relatively low vertical variability for the agricultural fields as revealed by (Dimitrova-Petrova et al., 2020a).

To determine the wetness conditions under which CRNS_{portable} sampling took place in contrasting SLU units, we explored different proxies for catchment wetness alongside topsoil point-scale SWC (θ_{SLU} and soil cores). These proxies included stream discharge at the catchment outlet (Q_{OUT}, in [mm day^{-1}]), the 7-day antecedent precipitation index (API_7, in [mm]) using daily precipitation data with a constant decay coefficient of 0.9 (Hooke, 1979), and the landscape-average soil water content estimated by the CRNS_{static} (SWC_{static} in [m^3 m^{-3}])
The latter also allowed for a more direct evaluation of the relative differences between SLU units and the CRNS<sub>static</sub> footprint. There were differences in soil properties between the static and portable sites, particularly in soil organic content, which was substantially greater at the MoorlandP unit. The procedure to account for those differences included a transformation of the CRNS<sub>static</sub> time series into synthetic time series of SWC for individual SLU units (SWC<sub>SLU</sub>) and testing the need for additional calibration of the shape parameters (a<sub>i</sub>) alongside N<sub>0</sub> in Equation 5, which represents the function used to transform neutron counts to SWC data.

\[
SWC_{SLU}(t) = \left(\frac{N_{SLU}(t)}{N_0 - a_1} - a_2\right) \times \rho_{dry} - (LW + SOM)
\]  

(Eq. 5)

for which SWC<sub>SLU</sub> is in [m<sup>3</sup> m<sup>-3</sup>], N<sub>SLU</sub> is in [cph], N<sub>0</sub> is the theoretical site-specific value of count rate over dry soil in [cph] (Desilets et al., 2010), and a<sub>i</sub> are shape coefficients. The ρ<sub>dry</sub> [g cm<sup>-3</sup>], LW [m<sup>3</sup> m<sup>-3</sup>] and SOM [m<sup>3</sup> m<sup>-3</sup>] are the estimated dry bulk density, lattice water and soil organic matter, respectively, as described above. The SWC<sub>SLU</sub> time series were additionally constrained. Total porosity was used as an upper limit, which meant that for SWC values above it, we assumed that the soils were saturated and any additional reduction in neutron counts was related to surface water ponding. Total porosity was estimated to be 0.6 for the managed SLU units and 0.8 for the MoorlandP. Lower SWC limit for the mineral SLU units was set to the minimum measured value at each unit (0.10 m<sup>3</sup> m<sup>-3</sup> in the CropP and 0.13 m<sup>3</sup> m<sup>-3</sup> in the PastureF, see Dimitrova-Petrova <em>et al.</em>, 2020b; 0.07 m<sup>3</sup> m<sup>-3</sup> at the CropI), while for the MoorlandP the lower SWC limit was set to 0.55 m<sup>3</sup> m<sup>-3</sup>, based on field knowledge on soil water retention and previous research on peaty podzols in Scotland (Tetzlaff <em>et al.</em>, 2014).

In most CRNS applications, typically only N<sub>0</sub> in Equation 5 is optimised, while all soil properties are determined from field observations (e.g. Evans <em>et al.</em>, 2016; McJannet <em>et al.</em>, 2016).
The shape coefficients of the equation are normally fixed at reference values of $a_0=0.0808 \text{[cm}^3\text{g}^{-1}]$, $a_1=0.372 \text{[-]}$, and $a_2=0.115\text{[cm}^3\text{g}^{-1}]$, derived by (Desilets et al., 2010) via neutron flux simulations for generic silica soils. However, some have identified the need for additionally calibrating the $a_i$ parameters to reproduce site-specific SWC dynamics or match local conditions (e.g. Iwema et al., 2015; Rasche et al., 2021; Rivera Villarreyes et al., 2011).

Here, we tested if such new calibration is needed to better fit field observations and hence allow consideration of site differences between SLU units, particularly in soil hydraulic properties and wetness dynamics, which is especially relevant for the peaty soils at MoorlandP.

For each SLU, we therefore tested two sensor calibration approaches based on the SWC data from the SLU to derive $\text{SWC}_{\text{SLU}}$ from $N_{\text{SLU}}$, while using the site specific $\rho_{\text{bulk}}$, LW, SOM, and SWC ($\theta_{\text{SLU}}$) data for Equation 5. More specifically, the first approach involved the typical standard $N_0$ calibration (Bogena et al., 2013), with fixed shape ($a_i$) parameters and optimization of only the $N_0$ parameter in Equation 5 (Table 2). In the second approach, referred here as new calibration, we simultaneously calibrated the $N_0$ and $a_i$ shape parameters. For this we used the Latin Hyper Cube approach (McKay, 1992) (Table 2). We performed 100 000 runs from which we obtained a single best parameter set, minimising the root mean square error (RMSE) and which fitted the field data best (i.e. daily averages of $N_{\text{SLU}}$ and field $\theta_{\text{SLU}}$ measurements on sampling days). The optimised parameters for each calibration were then used to solve Equation 5, producing two synthetic SWC timeseries per SLU unit, $\text{SWC}_{\text{typ}}$ and $\text{SWC}_{\text{new}}$, respectively.

To evaluate the new additional calibration of the shape parameters, we considered the potential improvement in fit to the data and the uncertainty around extremely wet or dry SWC estimates associated with the SWC constraints. We also calculated for each SLU unit the root mean square difference (RMSD) between the synthetic SWC timeseries produced with the typical and the new calibration, respectively (Equation 6).
In this equation, the $SWC_{typ,t}$ is mean soil water content estimate at time $t$, derived from $Ns_{SLU}$ using a SLU-specific $N_0$ and fixed $a_i$ parameters (Table 2). Correspondingly, $SWC_{new,t}$ is the soil water content derived from Equation 5, using the best parameter set of $N_0$ and $a_i$ from the Latin Hyper Cube simulations. A poor fit to the field data, a high proportion of unrealistic estimates using the standard approach, plus a relatively small RMSD all indicated the need for the additional calibration of the shape parameters to obtain SWC data. After the evaluation, only one time series $SWC_{SLU}$ (i.e. either the typical or new sensor calibration approach) per SLU unit was chosen for further calculations.

2.4. Spatially variable CRNS-derived near-surface storage ($S_{NS_{-}SLU}$) estimates for rainfall-runoff model calibration

The SWC data were then used to derive time series of near-surface water storage for the individual SLU units ($S_{NS_{-}SLU}$) and combine them with stream discharge in multi-criteria model calibration of a semi-distributed rainfall-runoff model for the catchment (objective iii). For that we used a semi-distributed version of the HBV-light model (Lindström et al., 1997; Seibert & Vis, 2012), which is a conceptual rainfall-runoff model that simulates discharge $Q_{sim}$ using a minimal input time series of precipitation ($P$), air temperature ($T$) and potential evapotranspiration ($PET$). The hydrological model comprises four main components: a snow (snow accumulation and melt), a soil (groundwater recharge and AET), a response (computes run-off as function of storage) and a routing (triangular weighting function for routing run-off to catchment outlet) routine (Seibert & Vis, 2012). The model was set up for Elsick at daily time steps using $P$, $T$ and PET input from 1 January 2011 to 31 December 2019, allowing for a relatively long warm-up period to eliminate the
effects of initial conditions, especially on storage. \(Q_{\text{OUT}}\) was available from 12 January 2015 to the end of the study period. While the effect of snow is accounted for, the parameters of the snow routine were fixed and not calibrated (see Supplementary Table 1), as snow contribution to precipitation in the catchment is minor. To simulate the presence of four SLU units in the catchment we opted for a model structure with four distributed soil zone reservoirs (SM) and the upper (SUZ) stores, while the lower model store (SLZ) was lumped. Each of the four SM and SUZ were given a weight corresponding to the proportion of the catchment covered by a specific SLU (Table 1), rescaled from a total of 94% catchment area to add up to 100%. While the SM represents the soil zone dynamics, the SUZ and SLZ roughly represent the shallow and deeper run-off generating stores, respectively. For Elsick, we conceptualised the HBV-light dynamic storage \(S_{\text{dyn}}(t)\) i.e. the storage activated in the runoff generation response as the sum of SM and SUZ at a given moment in time in each of the four semi-distributed stores. The rationale being that SM is responsible for the partitioning of precipitation input to deeper storage and ET, but does not produce runoff, while SUZ is the upper box that above a certain threshold (UZL parameter) generates \(Q_{\text{sim}}\). This combined storage is considered equivalent to the role of the near-surface soil water storage \((S_{\text{NS}})\), which the CRNS senses. On the other hand, the \(S_{\text{NS,static}}\) or \(S_{\text{NS,SLU}}\) represent the total water storage for a predetermined physical depth as opposed to \(S_{\text{dyn}}\), which, as in most conceptual rainfall-runoff models, is not bound to a specific depth. Therefore, a direct comparison of \(S_{\text{NS}}\) estimates \((S_{\text{NS,static}}\) or \(S_{\text{NS,SLU}}\)) with modelled storage dynamics \(S_{\text{dyn}}\) is not straightforward, here we opted for comparing the total soil column storage 0–400mm \((S_{\text{NS,SLU}})\) to \(S_{\text{dyn}}\), similar to Dimitrova-Petrova et al. (2020a).

To prepare storage data for the model calibration, we converted time series of \(\text{SWC}_{\text{static}}\) and \(\text{SWC}_{\text{SLU}}\) to \(S_{\text{NS,SLU}}\) using an exponential filter (as in Dimitrova-Petrova et al., 2020a) for the period 14 Nov 2015 – 31 December 2019. Next, the semi-distributed HBV-light rainfall-runoff model for the catchment was calibrated using the four \(S_{\text{NS,SLU}}\) as well as catchment \(Q_{\text{OUT}}\).
The model calibration period was 13 November 2015 to 31 December 2019 (~4 years). Days on which S_NS_SLU data were missing were not included in the model calibration. We used a Monte Carlo approach (100,000 independently generated parameter sets) for model calibration. Initial parameter ranges were set based on literature values (Seibert & Vis, 2012; Tetzlaff et al., 2015) and exploratory model runs (Supplementary Table 1). To account for model uncertainty, each model run was ranked according to the multiple-criteria (Pareto) ranking of model performance (following Rosolem et al., 2012). For each model run, this involved ranking of five criteria, which were the KGE goodness-of-fit (Kling-Gupta efficiency, Gupta et al., (2009)) of the Q_OUT to simulated discharge (KGE_Q_sim) and of the time series of S_NS_SLU to the corresponding simulated dynamic storage dynamics (KGE_Sdyn_SLU).

Consequently, we calculated the minimal Euclidian distance within the KGE space across the five criteria to select the best 50 parameter sets. As part of this, the five KGE criteria received different weights. A weight of 50% was assigned to the KGE of discharge (i.e. Q_sim), and 50% to the internal storage dynamics KGE_Sdyn_SLU, with weight proportional to their rescaled coverage of the SLU unit in the catchment. Equation 7 summarises the final multiple objective criteria (KGE_multiple) used here:

\[
KGE_{\text{multiple}} = \sqrt{0.5 \times (1 - KGE_{Q_{\text{sim}}})^2 + 0.18 \times (1 - KGE_{\text{Sdyn, Pasture}})^2 + 0.17 \times (1 - KGE_{\text{Sdyn, Crop1}})^2 + 0.24 \times (1 - KGE_{\text{Sdyn, Crop2}})^2}
\] (Eq. 7)

We also evaluated similarities and any differences in optimisations of identifiable parameters.

3. Results
3.1. Hydrometeorological and wetness conditions during study period

Continuous monitoring at Elsick spanned 1505 days (~ 4 years), covering a range of hydrometeorological conditions (Figure 2). The SWC_{CRNS} ranged between 0.14 at its driest and 0.6 at saturation (median was 0.37 $m^3$ $m^{-3}$). Observations at the CRNS_{static} started during an exceptionally wet winter in 2015-16, characterised by large precipitation events and floods (Figure 2 A). This was followed by a period of more seasonal wetting-drying cycles (March 2016 – June 2017). August 2017 – April 2018 was relatively wet and included a large rain on snow event in March 2018, which caused local flooding. The CRNS_{portable} surveys started during the summer of 2018, which was characterised by a prolonged streamflow recession and continuous soil drying, to capture the driest conditions observed at the catchment (Figures 2 C and C.1.). In the managed SLU units, average field SWC values, as measured with the theta probe ($\theta_{SLU}$ at depths 0-6 cm), were close to or slightly greater than SWC_{static}, while $\theta_{MoorlandP}$ was consistently much wetter. After subsequent rewetting, more surveys were conducted in all the SLU units during December 2018 – April 2019 and December 2019 to capture wetter soil conditions, respectively (Figures 2 C, C.2 and C.3). During these wetter soil conditions, average $\theta_{SLU}$ was greater at the CropP, PastureF and especially MoorlandP units as compared to SWC_{static}. During those periods, the field SWC at Cropl ($\theta_{Cropl}$ and soil cores) showed similar values to the SWC_{static} and the MoorlandP was consistently wetter, according to field measurements ($\theta_{Moorland}$ and soil cores). The $\theta_{SLU}$ spatial heterogeneity on each sampling day (indicated by standard deviations in Figure 2) was generally small but relatively large during dry and intermediate periods. During wet periods it was generally smaller and similar in all the SLU units, except for Cropl, for which was similar across all wetness conditions.

Field sampling of SWC in each SLU unit covered a similarly wide range of wetness conditions, as illustrated by comparing field SWC to three proxies of catchment wetness (Figure 3). Daily SWC_{static} displayed a strong linear relationship to the field SWC data in each
SLU unit (Figure 3 A). The managed SLU units within the static footprint (i.e. CropP and PastureF) were very well characterised, as sampling encompassed the 2\textsuperscript{nd} to the 93\textsuperscript{rd} percentiles of SWC\textsubscript{static}. The CropI and MoorlandP units outside the CRNS\textsubscript{static} footprint, were sampled under most wetness conditions, across the 3\textsuperscript{rd} and 60\textsuperscript{th} percentiles. Overall, the range of SWC measured in each managed SLU unit were similar to those in SWC\textsubscript{static}, while the MoorlandP was distinctly wetter. Field SWC data generally increased with API\textsubscript{7} and Q\textsubscript{OUT} (Figure 3 B and C, respectively). For variations with Q\textsubscript{OUT}, threshold behaviour was evident, which is in line with findings on storage – discharge relationships in the catchment, reported in Dimitrova-Petrova et al., (2020a).

3.2. Relationships between static and portable CRNS neutron data across SLU units

The cross-calibration of CRNS probes was carried out over five sampling days (Figure 2 C, C.1. and C.2.). Neutron intensities corrected for atmospheric influences from the two sensors, N\textsubscript{pih\_static} and N\textsubscript{pih\_portable}, respectively, related linearly (R\textsuperscript{2}=0.99), as shown in Figure 4 A. The mean ratio of 0.654 between them (Figure 4 B) was used to scale the neutron intensities of the CRNS\textsubscript{portable} (Equation 3). The sampling covered very dry to intermediate conditions, corresponding to very high (up to 99\textsuperscript{th} percentile of N\textsubscript{pih\_static}) and moderate neutron intensities (down to 40\textsuperscript{th} percentile of N\textsubscript{pih\_static}), respectively (Figure 4 A). The daily average SWC\textsubscript{static} on those days ranged between 0.17 to 0.37 m\textsuperscript{3} m\textsuperscript{-3} (2\textsuperscript{nd} to 50\textsuperscript{th} percentile of SWC\textsubscript{static}) and the average θ\textsubscript{static} (hand-held probe) ranged between 0.16 and 0.49 m\textsuperscript{3} m\textsuperscript{-3}. Thus the θ probe measurements seemed to overestimate soil moisture as compared to the CRNS SWC\textsubscript{static} during wet conditions, as it gives measurements at relatively shallower depths compared to the CRNS.
The scaled CRNS\textsubscript{portable} neutron intensity data ($N_{\text{SLU}}$) of each individual SLU unit showed a linear relationship ($R^2 > 0.5$) to the CRNS\textsubscript{static} neutron count data ($N_{\text{pih}_{\text{static}}}$), at a 4-hr integration time (Figure 5). The $R^2$ of that relationship ranged from 0.52 for CropP, and 0.79 to 0.98 for the remainder of the units. Consistent with the CRNS approach, the greatest neutron intensities corresponded with the driest sampling conditions (Figure 5, in red), while the least corresponded to wet or frozen soil conditions. There were subtle differences in the relationship of the SLU units within the CRNS\textsubscript{static} footprint (Figure 5 A, B). At the CropP unit (Figure 5 A), the $N_{\text{SLU}}$ data were more variable but close to $N_{\text{pih}_{\text{static}}}$. Such minimal differences relate logically to the fact that CropP unit occupies ~75% of the CRNS\textsubscript{static} footprint. For the PastureP unit (Figure 5 B), representing ~25% of CRNS\textsubscript{static}, there were even fewer notable differences between $N_{\text{SLU}}$ and $N_{\text{pih}_{\text{static}}}$. The CropI, situated outside the footprint of CRNS\textsubscript{static}, appeared to have generally greater neutron counts as compared to CRNS\textsubscript{static}, which was most pronounced during drier sampling conditions (Figure 5 C). At the wet MoorlandP unit neutron intensities were much lesser than $N_{\text{pih}_{\text{static}}}$ and also than any of the managed SLU units (Figure 5 D). The $N_{\text{SLU}}$ from the MoorlandP unit also seemed to experience relatively less variability in neutron counts, as evidenced by the smallest slope of the linear relationships in Figure 5.

3.3. Synthetic SWC timeseries for different Soil Land Use units

Soil property field data showed that the $\rho_{\text{bulk}}$ of the mineral soils (~1 g cm$^{-3}$) was much greater than for the organic-rich soil (0.28 g cm$^{-3}$), while SOM was six times less (Table 4). Moreover, the soil properties of all the mineral soil SLU units correspond with those in the CRNS\textsubscript{static} footprint. $N_0$ values for all SLU units used for the typical sensor calibration were greater, but all were within +15% of the $N_0$ for the static; differences being largest for the MoorlandP unit (Table 4).
Comparison between the typical and new calibration (Figure 6, in red and green, respectively) revealed that through the typical calibration, field data fitted reasonably well for the managed SLU units within the CRNS$_{\text{static}}$, CropP and PastureF (Figure 6 A and B, respectively). The new calibration was associated with no improvement in data fit and large RMSE, 0.033 and 0.035 m$^3$ m$^{-3}$, for the CropP and PastureF, respectively. Both typical and new sensor calibration produced a good fit to the data for the CropI unit, although the improvement in terms of reproducing the range of SWC using the new calibration was minimal (Figure 6 C, Table 4). In the case of the MoorlandP, only the new calibration produced realistic SWC dynamics (Figure 6 D, in green) with a good fit to the data, associated with the smallest RMSE (0.006 m$^3$ m$^{-3}$) (Table 4).

To produce the synthetic SWC timeseries, the typical calibration was kept for the managed SLU units, in- and outside the CRNS$_{\text{static}}$ footprint, and the additional parameter calibration was used solely for the MoorlandP unit. The timeseries of $N_{\text{SLU}}$ for each unit showed a similar range and overall dynamics to the CRNS$_{\text{static}}$ in the case of the managed SLUs (Figure 7 A). For the MoorlandP unit, neutron intensities were much lesser and showed less variability. This related to it being consistently wet, with fewer changes in SWC, compared to the managed units (Figure 7 B). Indeed, relative differences in terms of neutron intensity translated in similar patterns in terms of estimates for $\text{SWC}_{\text{SLU}}$ (Figure 7 B), effective sensing depth ($z_{\text{eff}}$) (Figure 7 C) and $S_{\text{NS}}$ (Figure 7 D). In terms of estimated $\text{SWC}_{\text{SLU}}$, the managed SLU units displayed a more dynamic behaviour, as compared to $\text{SWC}_{\text{static}}$. During dry conditions estimated $\text{SWC}_{\text{SLU}}$ values were close to the $\text{SWC}_{\text{static}}$ and much greater during intermediate and wet conditions (Figure 7 B). During the study period $z_{\text{eff}}$ of the CRNS$_{\text{static}}$ ranged between 7 and 18 cm (mean 11 cm), with $z_{\text{eff}}$ for the mineral SLU units again showing very similar mean and ranges. The $z_{\text{eff}}$ in the MoorlandP varied very little, being 7±1 cm, which relates to the reduced sensing depth of CRNS sensors when soils are wetter.
3.4. Comparison between near-surface soil water storage estimates (SNS) from individual SLU units and at the catchment-scale (for rainfall-runoff modelling input)

The two SLUs with crops showed very similar dynamics in SNS, while the PastureF was overall wetter than these other two mineral soils, especially during winter (Figure 7 D; Table 5). The MoorlandP generally followed the wetting and drying cycles but was much wetter than all of the mineral soil units and often saturated, consistent with field observations. Compared to the SNS_static, the SNS_SLU of the mineral SLU units showed greater variability (apart from the MoorlandP), and while all of the units were wetter on average, CropP and CropI were drier during dry periods (Table 5).

The outcomes of the multi-criteria calibration of the HBV-light semi-distributed for the Elsick catchment are shown in Figure 8 and their goodness of fit to observed data in Table 3. Overall, the model simulated discharge well across wetness conditions, except for the period April – October 2019, where Qsim was overestimated (Figure 8 A). The overall performance of the model calibrated using multiple criteria relates to the final parameter ranges (Supplementary Table 1). The 50 best parameter sets according to the multiple calibration criteria yielded median KGE_multiple of 0.51 and KGE_multiple ranged between 0.49 and 0.52. Across the five criteria KGE_Qsim ranged between 0.63 and 0.74 (median 0.70) (Table 3).

For these best 50 runs, the S_dyn was fairly well constrained for all of the SLU units and corresponded well with the observed storage dynamics (Figure 8 B, C, D, E). However, for Sdyn_CropP, calibrated on SNS_CropP data, the model overestimates the SNS during the dry period and then recovery, from April 2018 onwards (Figure 8 D). The uncertainty bands of the different S_dyn may additionally be related to the weight assigned to each KGE_Sdyn (Equation 7) i.e. narrower uncertainty band is related to a higher proportion of the weight assigned to a SLU unit. For example, Sdyn_CropI calibrated using SNS_CropI, which covers 37% of the catchment (Figure 8 C) shows much less uncertainty as compared to Sdyn_PastureF, calibrated...
on the $S_{\text{NS_PastureF}}$, which only covers 18\%. For the 50 best runs across the five criteria, the
median $KGE_{S_{\text{dyn}}}$ for the three mineral soils SLU units were similar, ranging between 0.33
and 0.40 and the median $KGE_{S_{\text{dyn_MoorlandP}}}$, calibrated on the organic-rich soil data was
0.31. For comparison, median $KGE_{S_{\text{dyn}}}$ when individual calibration criteria were used (data
not shown) varied between 0.43-0.50 for the mineral units and it was 0.38 for the MoorlandP.

Overall, final parameter ranges of the four $S_{\text{dyn}}$ were comparable, with a few exceptions.
Within the soil routine, the LP parameter which controls evaporation from the soil box was on
average higher in the $S_{\text{dyn_MoorlandP}}$, which related logically to the MoorlandP having more
available storage for evapotranspiration (Supplementary Table 1). Within the response
function, the $K0_{\text{MoorlandP}}$ and $K1_{\text{MoorlandP}}$ parameters, that are related to the outflow rate, were
relatively different for the $S_{\text{dyn_MoorlandP}}$ as compared to the $S_{\text{dyn}}$ of mineral soil SLUs. The
median $K0_{\text{MoorlandP}}$ related to the recession rate of quick flow was larger for the $S_{\text{dyn_MoorlandP}}$ as
compared to $S_{\text{dyn}}$ for the mineral soils, possibly relating to relatively less available soil
storage for runoff modulation (Supplementary Table 1). The median $K1_{\text{MoorlandP}}$ was relatively
lower, as compared to the mineral units, directly relating to the fact that the MoorlandP SLU
unit presents naturally poorer drainage in the upper layers.

4. Discussion

4.1. Using CRNS technology to explore relationships between soil
moisture dynamics of different soil-land use types

We explored the relationships between neutron intensities sensed within the static CRNS
footprint and those within key soil-land use units (objective (i)) using a combination of static
and portable CRNS sensors. The methodology we developed strived for an efficient
approach to characterise spatio-temporal SWC dynamics across different SLU units from
timeseries of static CRNS sensors. The need for a simple yet reliable way to relate soil
moisture datasets collected at different scales or with different spatial coverage is a key issue in hydrology and environmental modelling (Brocca et al., 2012; Pachepsky & Hill, 2017; Peters-Lidard et al., 2001; Peters-Lidard et al., 2017). Here we showed the potential of combining static and portable CRNS sensors to characterise distinct SLU units within a small (~10 km²) catchment. We made use of landscape representative neutron count and SWC timeseries from a static CRNS (Dimitrova-Petrova et al., 2020a) and related these to neutron measurements at key soil-land use units within the catchment, using a portable CRNS. This was combined with SLU-specific SWC and soil hydraulic properties information collected in the topsoil (0-6 cm).

Given that a representative location can be identified, many (data-intense) studies have found that under the same climate, point-scale time series of SWC at neighbouring sites can correlate well, despite contrasting soil, land use or topography (Lv et al., 2016; Mittelbach & Seneviratne, 2012; Zucco et al., 2014). Therefore, due to this commonly observed soil moisture temporal stability (Vachaud et al., 1985), it could be possible to use simple (linear) relationships to relate SWC dynamics at different locations and depths (Rosenbaum et al., 2012; Zhao et al., 2020), rescale SWC data, or use datasets from nearby locations for modelling purposes (Peterson et al., 2016; Seibert et al., 2011; Verrot & Destouni, 2016). This is on the condition that the spatial patterns and relationships between sites are known. There are also limitations with regards to the empirically derived linear relationships as these are unlikely to account for all localised short-term changes in SWC at individual SLU units. Nevertheless, applying these concepts to larger (field) scale patterns showed that such spatio-temporal information on near-surface soil water content can be obtained using CRNS technology. Ideally, this would be supported by a dense network of static CRNS sensors (as e.g. in Heistermann et al. 2021), although for most applications this would be unrealistic in terms of available resources. Our approach could therefore be proposed as a trade-off between the number of sensors and the requirements for continuous SWC estimates for key...
soil-land use units within the catchment. Considering that new cheaper detectors are becoming available on the market (e.g. Stevanato et al., 2019), we believe that our approach can be applied at locations where static CRNS are permanently installed and could extend to nearby ungauged catchments.

We demonstrated that the combined CRNS approach is well-suited to patchwork, mixed-agricultural landscapes which are characterised by spatially distributed farm fields with varying soil and land use properties (Hallett et al., 2016). In such context, installing and maintaining point-scale sensors is challenging due to soil management (e.g. harvesting, ploughing) as well as financial and access constraints (Vather et al., 2019; Dimitrova-Petrova et al., 2020a). The limited road network and generally wet soils make the use of a rover CRNS, impracticable. Such challenges can be tackled, as in the present study, by identifying key SLU units and complementing the static with a portable or “backpack” CRNS to assess spatial variability of near-surface soil water storage.

This initial assessment of the applicability of the combined CRNS approach was helpful both to address issues specific to the environment (wet climate and organic-rich soils, see section 4.2.), but also to identify future improvements. In this study, conversions from neutron count data to the synthetic SWC_{SLU} timeseries at the SLU units were supported by comprehensive ground truthing with a theta probe as well as soil sampling covering the CRNS footprints.

We found that the SWC spatial heterogeneity revealed by the theta probe SWC data within each SLU unit on each sampling day was relatively small. Nevertheless, soil agricultural management may introduce variations of soil hydraulic properties and hence soil moisture along the soil profile which may not be deducible from the SWC measured at the topsoil (Hupet & Vanclooster, 2002a; Wallace & Chappell, 2020). At the study site, this was only moderately evidenced. Soil sampling within the footprint revealed little variation in SWC with depth up to 30 cm during five calibration campaigns comprising a range of hydroclimatological conditions. A 30 min record of profile point-scale SWC measurements
next to the CRNS\textsubscript{static} (Dimitrova-Petrova et al., 2020a) also revealed that. For most of the
time, especially in wet periods, the topsoil showed similar SWC dynamics and magnitude to
lower depths (20 and 30 cm), although it was drier in intermediate and dry periods. In
addition to the fact that the impact on neutron signal strongly decreases with depth (Schrön
et al., 2017), we therefore limited our measurements in the other units to the top 5 cm of the
soil. Nevertheless, especially during drier conditions (Figure 7 C) and at drier sites (Franz et
al., 2012), the effective sensing depth of the CRNS technology can extend to 30 cm, which
should be considered in similar future studies. Additionally, the combination of theta probe
measurements with SWC information soil samples may not always lead to better
characterised relationships between SLU units (see Figure 3 A, where larger spread in SWC
data yields to lower R\textsuperscript{2} for two of the SLU units). Indeed, to better characterise the managed
SLU units using fewer points but with measurements of soil moisture deeper within the soil
profiles would help to improve the portable CRNS signal SWC estimates and reduce
uncertainty Baroni et al., (2018), while still sufficiently accounting for spatial heterogeneity.

Overall, more sampling would be recommended. Although the appropriateness of the linear
transformation was demonstrated by McJannet et al., (2017) in semi-arid Australian
landscape, sampling at intermediate wetness would then also allow to further evaluate and
refine the linear relationship between static and portable CRNS neutron counts in Elsick (as
shown in Figure 5). Most importantly, additional SWC information during intermediate
wetness conditions would help to better define the curve of the N-SWC relationship (as
shown in Figure 6). If these relationships could be characterised with more certainty, the
approach could then be applied in future sampling campaigns without more reliance on the
labour-intensive point scale measurements for sensor calibration.

Nevertheless, despite these uncertainties, using the combined CRNS approach we were
able to characterise SWC dynamics at all key SLU units in the Elsick catchment, including
the distinctly wetter MoorlandP SLU unit, which is generally more challenging to monitor.
(Bartalis et al., 2007; Tetzlaff et al., 2014). Differences between cropped sites (CropP and CropI) were found to be very small, likely due to the similar soil management they are subjected to (i.e. ploughing and presence of artificial soil drainage) (Boland-Brien et al., 2014; Hupet & Vanclooster, 2002). The PastureF was found to be the wettest managed SLU unit, with frequent surface ponding. Even though these soils are naturally freely draining, cattle grazing is thought to have caused compaction and thus greater water retention at the soil near-surface (Meyles et al., 2001; Wallace & Chappell, 2020). Similar conclusions were drawn at the study site using soil water isotope sampling and transit time modelling approaches (Dimitrova-Petrova et al., 2020b).

### 4.2. CRNS applications in humid environments

When creating synthetic time series of daily SWC for each SLU unit, our combined CRNS approach needed to account for site specific challenges i.e. the wet climate and presence of often saturated organic-rich soils (objective (ii)). The CRNS measurements have greater statistical uncertainty at lower neutron count rate, decreasing with longer integration time. This is specifically an issue in humid (Evans et al., 2016) and low-lying (Hawdon et al., 2014) catchments such as Elsick. To account for the uncertainty related to lower count rate, we deployed the portable CRNS at a single location representative for a SLU unit for 8 hours. This appeared as the only feasible option in this landscape, as opposed to using a rover CRNS. The generally more dynamic near-surface water storage estimates at the individual units ($S_{NS_{SLU}}$), as compared to the $S_{NS_{static}}$ are likely to be related to the inherently higher uncertainty in the wetter range of the N-SWC relationship and could also have been the result of SWC$_{SLU}$ overestimations during wet periods. On the other hand, the static CRNS was positioned at a location to provide integrated dynamics across several SLU units, therefore reflecting a more damped signal. This is reflected in the slope of the linear relationship between neutron counts of static and portable CRNS (Figure 5).
The presence of often saturated organic-rich (peaty) soils at Elsick, and many similar UK catchments (Lilly et al., 2015), posed additional challenges to the CRNS application. We identified that the moorland soils had distinct hydraulic properties, i.e. lesser bulk density, greater soil organic matter content and greater porosity (Bruneau & Johnson, 2014; Meyles et al., 2001; Tetzlaff et al., 2014), compared to the mineral soils. For sites with greater organic matter content, it has been shown that applying CRNS technology can indeed be challenging (Bogena et al., 2013; Fersch et al., 2018; Heidbuchel et al., 2016) and accounting for the effect of high organic matter on the CRNS signal often requires additional sampling effort (Jakobi et al., 2018; Vather et al., 2020). In organic-rich, near-saturated soils, using the reference (typical) Neutron Count-SWC (N-SWC) equation can lead to unrealistically dynamic SWC estimates. However, we showed that adequate characterisation could be easily achieved by additionally calibrating the shape (a) parameters determining the shape of the N-SWC relationship. We proposed the use of a simple and relatively easy to implement Latin Hypercube approach. This is consistent with findings for other CRNS applications which demonstrated the need of the additional a_i parameter calibration (Heidbuchel et al., 2016; Iwema et al., 2015; Rivera Villarreyes et al., 2011), although the needs for this should be evaluated locally (Iwema et al., 2015). While we sought the need to additionally calibrate the a_i parameter given the distinct soil hydraulic characteristics of the organic-rich soils, we do recognise that perhaps a more comprehensive soil sample dataset could reduce the uncertainty in the N-SWC for this SLU unit more.

While it might require the new sensor calibration, CRNS still has an advantage over point-scale measuring techniques in providing more spatially representative SWC estimates, overcoming spatial heterogeneity issues (Brunetti et al., 2019). Moreover, unlike other approaches (e.g. time domain reflectometry or TDR), the measurements are unaffected by temperature (Rivera Villarreyes et al., 2011) and due to the sensor design, lesser likely to be affected by saturation (overland flow, ponding).
Robust characterisation of SWC dynamics in humid landscapes has implications for flood and agricultural management. In particular, organic-rich peaty soils, which usually occupy the headwaters of many northern catchments (House et al., 2010), are both key to better understanding their distinct hydrological functioning (Boorman et al., 1995) and challenging to characterise with conventional techniques. In this study, the inclusion of the overall wetter MoorlandP SWC in the S\textsubscript{NS\_portable} estimates was logically related to the generally wetter areal average of SLU S\textsubscript{NS\_portable}, as compared to those observed with the static CRNS estimates alone. Additionally, the presence of moorlands on peaty soils in agricultural land bears multiple potential management benefits for farmers and policy makers including improved water quality and reducing the risk of erosion and flash flooding (Brown, 2020; Mcbride et al., 2017; RSPB, 2020). Thus, improved knowledge of their near-surface storage dynamics would be useful for management strategies, including flood warning applications.

### 4.3. How and when can spatially distributed information on near-surface soil water storage (S\textsubscript{NS}) help to calibrate rainfall-runoff models?

We derived time series of near-surface soil water storage CRNS (S\textsubscript{NS}) estimates for individual SLU units and demonstrated their added value for semi-distributed rainfall-runoff model calibration. Continuous time series of near-surface soil water storage CRNS (S\textsubscript{NS}) estimates at a landscape-representative location provide valuable information for improving subsurface parameterization in regional land surface models (Baatz et al., 2017) or rainfall-runoff model calibration (Dimitrova-Petrova et al., 2020a). This value can be enhanced if combined with “snapshots” of near-surface wetness variability from portable CRNS surveys, as demonstrated by Franz et al., (2015) and McJannet et al., (2017) from large scale experiments in dry climates. Our combined approach was applied at the small catchment scale to obtain continuous timeseries for different SLU units. It allowed identification of sites with wetter or more variable SWC dynamics, which can be missed if solely a landscape
average SWC value is used to characterise catchment S-Q relationships (Mittelbach & Seneviratne, 2012). The differences in near-surface soil water storage ($S_{NS}$) between mineral and organic-rich SLU units were captured by the combined CRNS approach and adequately constrained using an additional calibration of the N-SWC relationship.

While Dimitrova-Petrova et al. (2020a) previously demonstrated the value of the static CRNS $S_{NS}$ data in lumped rainfall-runoff model for Elsick, here we have expanded this to semi-distributed applications. Although not directly comparable (i.e. the calibration period in the present study was one year longer), the KGE median and ranges for discharge were similar using either the lumped or the semi-distributed HBV-light model set-up. However, in the semi-distributed approach here, the simulated discharge was better constrained as compared to using solely discharge or discharge and $S_{NS,\text{static}}$ and the internal catchment storage dynamics are arguably better represented. The $S_{NS,\text{static}}$ in the lumped model set-up did yield higher goodness of fit measures, but this could be simply related to the higher parameter uncertainty in the semi-distributed model due to having 36 parameters versus 15 in the lumped model set-up.

Ultimately, we have shown that CRNS technology provides a useful tool for semi-distributed, as well as lumped, rainfall-runoff modelling; and that the set-up will depend on whether the application requires a semi-distributed approach or not. Here, the semi-distributed HBV-light rainfall-runoff model served as a learning tool to investigate the role of near-surface storage and its spatiotemporal variation in the catchment-scale S-Q relationship. While the importance of $S_{NS}$ was evidenced by the improved model internal dynamics through the combined calibration (Dimitrova Petrova et al., 2020a), the additional effort associated with the combined static and portable CRNS approach for rainfall-runoff modelling yielded a relatively small gain in terms of simulated discharge. In this predominantly agricultural landscape, where land use managements (e.g. ploughing, artificial drainage) homogenises the soils at the near surface, data from the static CRNS installed at a landscape-
representative location appeared to sufficiently inform catchment-scale $S_{NS}$ dynamics (as demonstrated in Dimitrova-Petrova et al., (2020a)).

Further testing of the method in environments with contrasting climates and where spatial heterogeneity in $S_{NS}$ is more apparent will help evaluate whether deploying solely a static CRNS at a representative location in a catchment is sufficient or the combined approach could help to better characterise near-surface storage spatial heterogeneities. Another recommendation would be to test the use of CRNS in rainfall-runoff modelling in catchments with more pronounced seasonality. Such applications could help evaluate the trade-offs between the variable sensing depth of CRNS (Baroni et al., 2018; Peterson et al., 2016) and the usefulness of near-surface storage data to characterise catchment storage dynamics and potentially improve flood forecasting (Massari et al., 2014; Massari et al., 2018).

Although not yet applied to hydrological modelling, similar but more data intense CRNS studies in drier agricultural landscapes (Gibson & Franz, 2018; McJannet et al., 2017) have successfully assessed spatiotemporal dynamics of near-surface storage. While distributed soil management poses additional challenges in mixed-agricultural environments, a combined CRNS approach complemented with a few continuous point-profile measurements could help elucidate the wider applicability of the approach and increase its information value along the SWC profile (Scheiffele et al., 2020). In addition, more complex models more sensitive to storage might benefit even more from the spatially variable $S_{NS}$ information produced using the combined static and portable CRNS data approach.

5. Conclusions

We combined static and portable CRNS sensors to assess the spatial variability of near-surface soil water storage dynamics in a small (10km$^2$) humid mixed-agricultural catchment. For that, we developed and tested a method suited to this environment, which extends the information content of static CRNS to key soil-land use units. We demonstrated that the
approach worked well to characterise SWC dynamics at all key SLU units in the Elsick study catchment, although recommend careful consideration of additional SWC calibration data that accounts for spatial variability in depth as well as within the CRNS footprint. Within our approach we also addressed landscape-specific CRNS related challenges. Firstly, much longer integration time of neutron counts (~4 hours), compared to temperate and semi-arid sites, were needed to account for high neutron uncertainty. Secondly, this study identified the need for additional parameter calibration of the SWC CRNS function for characterising SLU units with contrasting soil hydraulic properties. Here this involved the Moorland on organic-rich poorly drained soils, typical for this and many other humid landscapes. We then tested the value of the new spatially variable SWC catchment data for the catchment for a semi-distributed rainfall-runoff model calibration, in comparison to simulations using just the static CRNS data in a previous study. Based on minimal differences in model efficiency and simulated runoff we conclude that (i) data from static CRNS at a landscape-representative location might suffice to inform rainfall-runoff modelling at the small (1-10 km²) catchment scale (ii) depending on the research needs and objectives a (semi-)distributed model structure might be useful in heterogeneous environments, but not strictly necessary. This preliminary study shows the potential of combining CRNS technologies to assess spatiotemporal variability of near-surface water storage in humid agricultural landscapes. It also encourages further investigations in environments with contrasting climate or pronounced seasonality to improve its accuracy and applicability. Depending on model structure and the degree to which near-surface storage dynamics vary within the landscape, such datasets can improve storage-discharge relationships, flood and agricultural management applications in humid landscapes.
Acknowledgements

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References


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Lilly, Allan, Miller, D., Towers, W., Donnelly, D., Poggio, L., & Carnegie, P. (2015). MAPPING SCOTLAND ’ S SOIL RESOURCES, 48(Figure 2), 35–46.


Research, 55(6), 4785–4800. https://doi.org/10.1029/2018WR024535


Table 1. Distribution of soil-land use (SLU) classes in the Elsick catchment. In bold the classes represented by the CRNS\textsubscript{portable} sampling (covering 94% of the catchment).

<table>
<thead>
<tr>
<th>Soil land use (SLU) class</th>
<th>%</th>
<th>%</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>CRNS\textsubscript{static}</td>
<td>Elsick</td>
</tr>
<tr>
<td><strong>Crop – Imperfectly drained (CropI)</strong></td>
<td>-</td>
<td>35%</td>
</tr>
<tr>
<td>Rotational crops on imperfectly drained podzols</td>
<td>-</td>
<td>35%</td>
</tr>
<tr>
<td><strong>Crop – Poorly drained (CropP)</strong></td>
<td>75%</td>
<td>32%</td>
</tr>
<tr>
<td>Rotational crops on poorly drained gleys</td>
<td>75%</td>
<td>32%</td>
</tr>
<tr>
<td><strong>Pasture – Freely drained (PastureF)</strong></td>
<td>25%</td>
<td>17%</td>
</tr>
<tr>
<td>Pasture on freely drained podzols</td>
<td>25%</td>
<td>17%</td>
</tr>
<tr>
<td><strong>Moorland- Poorly drained (MoorlandP)</strong></td>
<td>-</td>
<td>10%</td>
</tr>
<tr>
<td>Moorland and woodland on poorly drained peats and peaty podzols with organic-rich surface layer</td>
<td>-</td>
<td>10%</td>
</tr>
<tr>
<td>Others (Forest plantations on mineral soils)</td>
<td>-</td>
<td>4%</td>
</tr>
<tr>
<td>Suburban and quarries</td>
<td>-</td>
<td>&lt;2%</td>
</tr>
<tr>
<td>Open Water</td>
<td>-</td>
<td>&lt;1%</td>
</tr>
</tbody>
</table>
Table 2. Initial parameter ranges of the two CRNS calibration approaches tested for deriving synthetic \( \text{SWC}_{\text{SLU}} \) timeseries from the combined CRNS dataset.

<table>
<thead>
<tr>
<th>Calibration (SWC)</th>
<th>( N_0 )</th>
<th>( a_0 )</th>
<th>( a_1 )</th>
<th>( a_2 )</th>
<th>Initial parameter range ( a_i )</th>
<th>Initial parameter range ( N_0 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Typical (SWC\text{typ})</td>
<td>calibrated</td>
<td>fixed</td>
<td>fixed</td>
<td>fixed</td>
<td>-</td>
<td>Fixed</td>
</tr>
<tr>
<td>New (SWC\text{new})</td>
<td></td>
<td></td>
<td>calibrated</td>
<td>calibrated</td>
<td>calibrated</td>
<td>( N_{0,\text{static}} = a_0 = [0 \ 1] [\text{cm}^3 \text{g}^{-1}] )</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>( a_1 = [0 \ 1] [-] )</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>( a_2 = [0 \ 1] [\text{cm}^3 \text{g}^{-1}] )</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>( 3450 \text{ cph} \pm 10% )</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>( a_2 = [0 \ 1] [\text{cm}^3 \text{g}^{-1}] )</td>
</tr>
</tbody>
</table>
Table 3. Overview statistics (median, minimum and maximum) of the goodness of fit of the 50 best model runs. Both the multiple criteria $KGE_{\text{multiple}}$ as well as the individual KGE measures are presented.

<table>
<thead>
<tr>
<th>Goodness of fit Median [Min Max]</th>
<th>Calib.target</th>
</tr>
</thead>
<tbody>
<tr>
<td>$KGE_{\text{multiple}}$</td>
<td>0.51 [0.49-0.52]</td>
</tr>
<tr>
<td>$KGE_{Q_{\text{sim}}}$</td>
<td>0.70 [0.63-0.74]</td>
</tr>
<tr>
<td>$KGE_{{S_{\text{dyn, PastureF}}}}$</td>
<td>0.40 [0.25-0.49]</td>
</tr>
<tr>
<td>$KGE_{{S_{\text{dyn, Cropl}}}}$</td>
<td>0.36 [0.24-0.43]</td>
</tr>
<tr>
<td>$KGE_{{S_{\text{dyn, CropP}}}}$</td>
<td>0.33 [0.25-0.42]</td>
</tr>
<tr>
<td>$KGE_{{S_{\text{dyn, MoorlandP}}}}$</td>
<td>0.31 [0.22-0.37]</td>
</tr>
</tbody>
</table>
Table 4. Overview of soil characteristics (bulk density $\rho_{dry}$, soil organic matter SOM and lattice water LW) and calibrated parameters using the typical or the new sensor calibration for each SLU unit. For the typical one, $a$ parameters are fixed ($a_0=0.0808$, $a_1=0.372$ and $a_2=0.115$, Desilets et al., 2010). For the new calibration all four parameters are calibrated. RMSE (fit to field data) is also reported.

<table>
<thead>
<tr>
<th>Soil Land Use</th>
<th>$\rho_{dry}$ [g cm$^{-3}$]</th>
<th>SOM + LW [m$^3$ m$^{-3}$]</th>
<th>Typical calibration</th>
<th>New ($N_0 + a_i$) calibration</th>
<th>RMSE [m$^3$ m$^{-3}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Static</td>
<td>1.09</td>
<td>0.07</td>
<td>3450 (1)</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>CRNS</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CropP</td>
<td>1.13</td>
<td>0.07</td>
<td>3510</td>
<td>3610</td>
<td>0.326 0.278 0.944 0.033</td>
</tr>
<tr>
<td>PastureF</td>
<td>0.98</td>
<td>0.07</td>
<td>3720</td>
<td>3214</td>
<td>0.521 0.194 0.83 0.035</td>
</tr>
<tr>
<td>CropI</td>
<td>1.1</td>
<td>0.07</td>
<td>3680</td>
<td>3490</td>
<td>0.076 0.432 0.202 0.014</td>
</tr>
<tr>
<td>MoorlandP</td>
<td>0.28</td>
<td>0.41</td>
<td>3910</td>
<td>4332</td>
<td>0.938 0.117 0.0974 0.006</td>
</tr>
</tbody>
</table>
Table 5. Overview statistics of near-surface soil water storage ($S_{NS}$) estimates from the static CRNS and individual SLU units (considered $S_{NS}$ timeseries for rainfall-runoff modelling in bold).

<table>
<thead>
<tr>
<th>$S_{NS}$ (mm)</th>
<th>Static $S_{NS_{static}}$</th>
<th>CropP</th>
<th>PastureF</th>
<th>CropI</th>
<th>MoorlandP</th>
</tr>
</thead>
<tbody>
<tr>
<td>Min</td>
<td>66</td>
<td>44</td>
<td>70</td>
<td>69</td>
<td>48</td>
</tr>
<tr>
<td>Mean</td>
<td>150</td>
<td>164</td>
<td>204</td>
<td>197</td>
<td>164</td>
</tr>
<tr>
<td>Median</td>
<td>151</td>
<td>165</td>
<td>215</td>
<td>205</td>
<td>165</td>
</tr>
<tr>
<td>Max</td>
<td>219</td>
<td>240</td>
<td>240</td>
<td>240</td>
<td>240</td>
</tr>
<tr>
<td>SD</td>
<td>27</td>
<td>47</td>
<td>37</td>
<td>36</td>
<td>40</td>
</tr>
<tr>
<td>NA</td>
<td>5</td>
<td>37</td>
<td>6</td>
<td>28</td>
<td>5</td>
</tr>
</tbody>
</table>
Figure 1. The Elsick catchment and instrumentation, showing (a) the soil-land use (SLU) units distribution and overview of the permanent and temporary monitoring infrastructure i.e. location of the gauging stations, $CRNS_{\text{static}}$ and $CRNS_{\text{portable}}$ sensor sampling; (b) zoom of the $CRNS_{\text{static}}$ location (yellow star) and footprint, covering two SLU units and soil sampling locations for sensor calibration. The white stars and circumference indicate the locations where portable CRNS was deployed and distributed topsoil (0-6 cm) SWC measurements were taken within its footprint; (c) the static (i.e. permanently installed) CRNS-weather station and portable CRNS; (d) to (g) show sampling locations of individual SLU units: (d) PastureF; (e) CropP; (f) CropI and (g) MoorlandP.
Figure 2. Timeseries of P, Q_{OUT}, PET and SWC_{static} for the period 14 November 2015 to 31 December 2019. Panel C highlights in blue the three specific periods during which CRNS_{portable} sampling took place. Daily depth-distance weighted averages of field SWC sampled using theta probe (diamond) or soil samples (circles) at each SLU unit are also shown, standard deviation (SD, as error bars) also shown. CRNS_{static} calibration includes soil samples taken at the PastureF and CropP SLU units. Panels C1 to C3 zoom in those periods. Sampling days on which soils were frozen are indicated with X in panel C and C2.
Figure 3. Overview of the relationships of topsoil SWC (either theta probe $\theta_{SLU}$ or soil cores information) the four SLU units to proxies of catchment wetness dynamics (a) $\text{SWC}_{\text{static}}$; (b) API, and (c) $Q_{\text{OUT}}$. Daily averages of SWC$_{\text{static}}$ (grey circles) are also plotted against API and $Q_{\text{OUT}}$ (Figure 3 B and C, respectively) for context. Boxplots on the right-hand side illustrate the range of the field SWC data.
Figure 4. CRNS sensors cross-calibration A) Scatterplot showing correlation between the scaled corrected counts of portable CRNS ($N_{pih_{portable}}$) versus static CRNS ($N_{pih_{static}}$) within the footprint of the permanently installed sensor. B) Boxplots showing the spread of the ratio Portable/Static CRNS for 4hrs integration times and the mean of the ratios (0.654, in red) (median shown as the thick black line of the boxplot).
Figure 5. Relationship between static and portable CRNS data derived from neutron counts corrected for atmospheric influences, in the case of the portable (NsSLU) and additionally corrected for the effect of vegetation in the case of the static (Npihv). For integration times of 4h, all scaled to 1h (cph). Each subplot corresponds to an individual soil-land use unit. In brackets the weighted volumetric SWC (θdw in m$^3$ m$^{-3}$) measured in the field using the θ probe. The colours of the dots indicate whether the field soil moisture was considered dry (red), intermediate (green) or wet (dark blue) or if the topsoil was...
frozen (light blue). Error bars correspond to the coefficient of variance (CV). Black line represents the trendline of the linear regression \((y=ax+b)\). Grey line represents a 1:1 relationship.

Figure 6. The \(N_{\text{phv}}{}^\text{static}-\text{SWC}\) relationship for the static CRNS (black) and the \(N_{S}\_\text{SLU}-\text{SWC}\) synthetic timeseries, using typical (in red) and new (in green) sensor calibration together with the field data tested.
Figure 7. Portable SWC and related variables: overview A) Daily average Npihv for CRNS\textsubscript{static} and \(N_s\)\textsubscript{SLU} for each individual SLU units. B) SWC for the CRNS\textsubscript{static} and synthetic estimates SWC\textsubscript{SLU} of...
individual SLU units; C) Effective depth ($z_{\text{eff}}$) of CRNS and estimates for individual SLU units; d) Estimated $S_{\text{NS}}$ (in mm) for with CRNS\textsubscript{static} and $S_{\text{NS,SLU}}$ for individual units.
Figure 8. Semi-distributed rainfall-runoff modelling outcomes. Panel A show the time series of incoming precipitation $P$ and the time series of observed $Q_{OUT}$, median (in red) and uncertainty bands (in grey) of $Q_{sim}$ of the best 50 runs using a multiple-criteria calibration approach i.e. combining $S_{NS\_SLU}$ and $Q_{OUT}$ as model calibration targets. Panel B to E show the simulated dynamic storage $S_{dyn}$ and corresponding the $S_{NS\_SLU}$ data used for its calibration. The median (in red) and uncertainty bands (in grey) of the best 50 runs in also displayed. Pareto ranking of ($KGE_{multiple}$, Eq. 7) used as a goodness of fit measure.
### Appendix I  Definitions of storage and related terms.

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Units</th>
<th>Definition</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>CRNS</td>
<td>[-]</td>
<td>Cosmic ray neutron sensor</td>
<td>Hydroinnova, New Mexico</td>
</tr>
<tr>
<td>CRNS\textsubscript{static}</td>
<td>[-]</td>
<td>A static cosmic ray neutron sensor installed in a permanent location</td>
<td>This study</td>
</tr>
<tr>
<td>CRNS\textsubscript{portable}</td>
<td>[-]</td>
<td>A portable cosmic ray neutron sensor which can be moved to different locations. Applications include rover (mounted on a vehicle), backpack (carried on a field operator’s back). The current study uses the suitcase or cross-calibrator version of Hydroinnova.</td>
<td>(Dong et al., 2014; Franz, 2018; Hydroinnova, 2020)</td>
</tr>
<tr>
<td>N\textsubscript{raw}</td>
<td>[cph]</td>
<td>Cosmic ray neutron intensity as measured by the CRNS, in neutron counts per hour [cph],</td>
<td>This study</td>
</tr>
<tr>
<td>N\textsubscript{pih(v)}</td>
<td>[cph]</td>
<td>Cosmic ray neutron intensity measured as neutron counts per hour [cph], inversely correlated to all hydrogen present in the upper decimetres of the subsurface and the first few hectometres of the atmosphere above the ground surface. The N signal is corrected for effects of atmospheric pressure (p), incoming neutron flux (i), air humidity (h) and in some cases the effect of aboveground vegetation (v)</td>
<td>(Baatz et al., 2015; Zreda et al., 2012; Zreda et al., 2008)</td>
</tr>
<tr>
<td>N\textsubscript{pih\textsubscript{v}}\textsubscript{static}</td>
<td>[cph]</td>
<td>N\textsubscript{pih\textsubscript{v}}, as defined above, derived from data obtained with the static CRNS</td>
<td>(Baatz et al., 2015; Zreda et al., 2012; Zreda et al., 2008)</td>
</tr>
<tr>
<td>N\textsubscript{pih\textsubscript{portable}}</td>
<td>[cph]</td>
<td>N\textsubscript{pih}, as defined above, derived from data obtained with the portable CRNS</td>
<td>(Baatz et al., 2015; Zreda et al., 2012; Zreda et al., 2008)</td>
</tr>
<tr>
<td>N\textsubscript{s, portable}</td>
<td>[cp4h]</td>
<td>N\textsubscript{pih\textsubscript{portable}} (up) scaled by a known ratio, so that portable matches the magnitude/potency of the static CRNS data. Used to define the relationship between portable and static CRNS data via linear regression</td>
<td>This study</td>
</tr>
<tr>
<td>Variable</td>
<td>[Unit]</td>
<td>Description</td>
<td>Source</td>
</tr>
<tr>
<td>----------</td>
<td>--------</td>
<td>-------------</td>
<td>--------</td>
</tr>
<tr>
<td>(N_{\text{SLU}}(t))</td>
<td>[cph]</td>
<td>Synthetically derived time series of neutron intensity derived for an individual soil-land use unit within the catchment, from time series of (N_{\text{pih,static}}), based on the linear relationship between (N_{\text{sl, portable}}) and (N_{\text{pih,static}}).</td>
<td>This study</td>
</tr>
<tr>
<td>(Z_{\text{eff}}(t))</td>
<td>[cm]</td>
<td>Estimated effective sensing depth of the CRNS at time (t), a function of SWC, bulk density and soil organic matter (SOM).</td>
<td>(add ref from methods)</td>
</tr>
<tr>
<td>(\text{SWC}_{\text{static}})</td>
<td>([\text{m}^3 \text{m}^{-3}])</td>
<td>Field average (~14 ha) soil water content based on calibrated static Cosmic Ray Neutron Sensor data; integrated over a time-variable sensing depth (Z_{\text{eff}}) (between 0.07 and 0.2 m).</td>
<td>(Schrön et al., 2017; Zreda et al., 2008)</td>
</tr>
<tr>
<td>(\text{SWC}_{\text{typ}})</td>
<td>([\text{m}^3 \text{m}^{-3}])</td>
<td>Synthetically derived time series of field average soil water content using a typical sensor calibration ((N_0) parameter) for an individual soil-land use unit within the catchment; integrated over a time-variable sensing depth (Z_{\text{eff}}).</td>
<td>This study</td>
</tr>
<tr>
<td>(\text{SWC}_{\text{new}})</td>
<td>([\text{m}^3 \text{m}^{-3}])</td>
<td>Synthetically derived time series of field average soil water content using a new sensor calibration ((N_0) and (a_i) parameters) for an individual soil-land use unit within the catchment; integrated over a time-variable sensing depth (Z_{\text{eff}}).</td>
<td>This study</td>
</tr>
<tr>
<td>(\text{SWC}_{\text{SLU}})</td>
<td>([\text{m}^3 \text{m}^{-3}])</td>
<td>Synthetically derived time series of field average soil water content for individual soil-land use unit within the catchment; integrated over a time-variable sensing depth (Z_{\text{eff}}). The SWC values are derived using either typical or new sensor calibration of the neutron intensity.</td>
<td>This study</td>
</tr>
<tr>
<td>(\theta_{\text{SLU}})</td>
<td>([\text{m}^3 \text{m}^{-3}])</td>
<td>The arithmetic average of the theta (\theta) probe measurements on each sampling day, used to characterise the CRNS signal and to account for point scale spatial variability of SWC within the footprint on that day.</td>
<td>(Delta T Devices Ltd.)</td>
</tr>
</tbody>
</table>
This study (Dimitrova-Petrova et al., 2020a)

SNS [mm] Near-surface storage for a defined depth (z=0.4 m)

This study

SNS_static [mm] Near-surface storage for a defined depth (z=0.4 m) determined as the sum of SWC\textsubscript{static} and SWC\textsubscript{static\_SLU}

This study

SNS\_SLU [mm] Near-surface storage for a defined depth (z=0.4 m) determined as the sum of SWC\textsubscript{SLU} and SWC\textsubscript{SLU\_sub}

This study

S\textsubscript{dyn\_SLU} [mm] Dynamic Storage (catchment scale), considered to control the majority of streamflow response. In the selected model structure set-up, it is the sum of the storage in the SM (soil moisture) and the SUZ (upper groundwater zone) boxes in the semi-distributed set-up of the HBV-light model. The indices correspond to the SLU units, data from which (S\textsubscript{NS\_SLU}) was used to calibrate each of the four dynamic storage boxes.

This study

SM [mm] HBV model: Soil moisture box with its largest value equal to FC (field capacity). Partitioning of rainfall in soil water content and groundwater recharge. Does not produce runoff

(Seibert, 2005)

SUZ [mm] HBV model: Upper groundwater box, recharged by the SM box. Faster runoff (Q\textsubscript{0}) of the SUZ box depends on the UZL (upper zone limit) parameter which acts as a threshold above which runoff is produced. Slower runoff Q\textsubscript{1} from this box depends on K1 recession constant.

(Seibert, 2005)

SLZ [mm] Lower groundwater box (PERC in mm day\textsuperscript{-1} defines the max percolation rate from the upper to the lower groundwater box)

(Seibert, 2005)
Supplementary Table 1. Initial and final parameter ranges for the multi-criteria model calibration using synthetically derived CRNS S_{NS,SLU} of four SLU units together with observed discharge of the best 50 runs. Parameters Pcorr=1, TT=0, CFMAX=1, CET=1, CFR=0.05, CWH=1 were fixed.

<table>
<thead>
<tr>
<th>Soil Routine</th>
<th>Lower limit</th>
<th>Upper limit</th>
<th>Median [Min Max]</th>
<th>Response function</th>
<th>Lower limit</th>
<th>Upper limit</th>
<th>Median [Min Max]</th>
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<tbody>
<tr>
<td>BETA_PastureF</td>
<td>1</td>
<td>6</td>
<td>2.5 [1.1-5.5]</td>
<td>K0_PastureF</td>
<td>0.1</td>
<td>0.8</td>
<td>0.36 [0.13-0.8]</td>
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<tr>
<td>BETA_CropI</td>
<td>1</td>
<td>6</td>
<td>3.5 [1.3-5.9]</td>
<td>K0_CropI</td>
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<td>0.8</td>
<td>0.42 [0.11-0.78]</td>
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<tr>
<td>BETA_CropP</td>
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<td>6</td>
<td>3.2 [1.1-5.9]</td>
<td>K0_CropP</td>
<td>0.1</td>
<td>0.8</td>
<td>0.41 [0.14-0.77]</td>
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<tr>
<td>BETA_MoorlandP</td>
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<td>4</td>
<td>2.5 [1-3.6]</td>
<td>K0_MoorlandP</td>
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<td>0.8</td>
<td>0.55 [0.15-0.8]</td>
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<tr>
<td>FC_PastureF</td>
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<td>500</td>
<td>318 [50-446]</td>
<td>K1_PastureF</td>
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<td>0.63 [0.22-0.79]</td>
</tr>
<tr>
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<td>235 [126-477]</td>
<td>K1_CropI</td>
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<td>0.8</td>
<td>0.59 [0.07-0.8]</td>
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<tr>
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<td>246 [182-327]</td>
<td>K1_CropP</td>
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<td>0.8</td>
<td>0.67 [0.08-0.79]</td>
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<tr>
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<td>500</td>
<td>318 [210-460]</td>
<td>K1_MoorlandP</td>
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<td>0.8</td>
<td>0.54 [0.18-0.8]</td>
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<tr>
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<td>0.5 [0.3-1]</td>
<td>K2</td>
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<td>0.1</td>
<td>0.054 [0.007-0.098]</td>
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<td>MAXBAS</td>
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<td>1.4 [1-2.3]</td>
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<td>1</td>
<td>0.4 [0.3-1]</td>
<td>PERC_PastureF</td>
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<td>1.2 [0.2-3.6]</td>
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<td>4</td>
<td>1.1 [0-3.7]</td>
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<tr>
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<td>34 [7-65]</td>
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<tr>
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<td>43 [7-69]</td>
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</table>