Accuracy and precision of the cosmic-ray neutron sensor for soil moisture estimation at humid environments

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Abstract
The accuracy and precision of the cosmic-ray neutron sensor (CRNS) neutron count and soil moisture estimate are affected differently by distinct neutron moderating factors. Moreover, whereas the accuracy can be improved by correcting for different hydrogen pools, the precision can only be improved by increasing the surface area of the CRNS sensors or by increasing the integration time. To date, the effects of different neutron moderating factors on CRNS accuracy and precision are not completely understood. We used data from three agricultural and low biomass sites located within a few kilometres distance from each other in South England. We developed an extended version of the COsmic-ray Soil Moisture Interaction Code (COSMIC), which included the effects of relevant neutron moderating factors on the neutron counts. With sensitivity analysis, we found atmospheric pressure and soil moisture content to be most influential on neutron count accuracy and precision. These two factors were, respectively, seven and four times more important than soil bulk density, lattice water and soil organic matter. Above ground biomass was substantially less influential compared to these variables. However, because the three sites had similar soil organic matter and meteorology, calibration results showed that differences between sites could be mostly explained by differences in above ground biomass and to a lesser extent intercepted water. The neutron count differences due to above ground biomass corresponded with substantial soil moisture estimate differences up to 0.07 cm\(^3\)/cm\(^3\); a significant effect on soil moisture accuracy. The precision of the soil moisture estimate was 10 times more sensitive to soil moisture than other factors and was therefore mostly a function of soil moisture content itself. The neutron count integration times required to obtain a soil moisture precision were typically less than a day. Our results are indicative for other humid, temperate, agricultural sites.

Keywords
agricultural sites, COSMIC, cosmic-ray neutron sensor, measurement accuracy, measurement precision, parameter calibration, sensitivity analysis, soil moisture

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1 | INTRODUCTION

Soil moisture is a key factor in the redistribution of both water and energy at the land surface and is a valuable ecohydrological resource (Robinson et al., 2008). Moreover, soil moisture also plays a role in climate change processes (Entekhabi, 1995; Seneviratne et al., 2006), biogeochemical processes (Robinson et al., 2008; Seneviratne et al., 2010), the quantity and quality of available water in ecosystems and the transport of chemicals and nutrients (Robinson et al., 2008; Siebert et al., 2005). As a crop water resource, soil moisture is a central factor in agriculture and therefore in feeding the human population. In order to better understand the role soil moisture plays, and to make relevant predictions, soil moisture observations at intermediate scales are needed (Robinson et al., 2008; Vereecken et al., 2008, 2015).

The cosmic-ray neutron sensor (CRNS) estimates soil moisture content at sub-kilometre scale by measuring epithermal neutron radiation interactions with soil and its surroundings (Baatz et al., 2014; Bogena et al., 2013; Evans et al., 2016; Hawdon et al., 2014; Rivera Villarreyes et al., 2011; Zreda et al., 2008; Zreda et al., 2012). The main advantage of the CRNS compared to more traditional soil moisture sensing techniques is its spatial scale with a horizontal footprint of a few hundreds of metres (Desilets & Zreda, 2013; Franz et al., 2012a; Köhli et al., 2015). In addition, the CRNS' effective depth can reach a few tens of centimetres with a temporal resolution from minutes to days, depending on the measurement integration time (Bogena et al., 2013; Zreda et al., 2008). Previous studies showed excellent agreement between CRNS-estimated soil moisture in comparison to co-located point-scale sensor networks covering a similar footprint, at sites with advantageous conditions (root mean square deviation, RMSD, in the order of 0.01 cm$^3$ cm$^{-3}$; Franz et al. (2012a); Schreiner-Mcgraw et al. (2016); Zhu et al. (2016)).

However, at sites with less advantageous conditions (for instance high atmospheric pressure, high biomass density, humid climate), lower performance has been found (Bogena et al., 2013; Coopersmith et al., 2014; Franz et al., 2016; Sigouin et al., 2016; Zhu et al., 2015). These less advantageous conditions are characterized by sites with higher abundance of other environmental factors than soil moisture that affect the measured neutron intensity (Zreda et al., 2012). The first reason is that hydrogen has especially strong stopping and slowing-down power to cosmic-ray neutrons (Zreda et al., 2008). The CRNS measures the epithermal neutron radiation by counting the number of these neutrons entering the neutron counter (tube). Therefore, other materials can be a source of hydrogen, including biomass (Baatz et al., 2015), lattice water (Desilets et al., 2010; Zreda et al., 2012), soil organic matter (Franz et al., 2013) and atmospheric water (Rosolem et al., 2013) eventually affect the CRNS measurements. Secondly, other effects not necessarily related to sources of hydrogen such as the intensity of the incoming cosmic rays (Blasi, 2014; Desilets & Zreda, 2001) and their attenuation within the atmosphere (Zreda et al., 2012) also influence the CRNS measurement.

Accuracy and precision are two distinct performance metrics. Accuracy is a measure of how close the average of multiple estimates is to the target (or truth). Precision of a measurement is the consistency in making multiple measurements under the same conditions, that is, how close the different estimates are to one another. The precision is often quantified with the standard deviation. The CRNS accuracy and precision can both be improved in different ways. To improve the accuracy, corrections for the effects of moderating factors other than the target variable (soil moisture) are needed. The precision can however only be improved by increasing the number of neutrons counted from which a soil moisture estimate is derived. This can be achieved by installing a more efficient sensor, increasing the surface area of the sensor (i.e., a larger single CRNS tube or co-locating multiple CRNS tubes), or by increasing the neutron count integration time. Due to the different natures of both the CRNS accuracy and precision, separating them can help in further development and application of the sensor technique. In addition, separate information on the accuracy and precision can be relevant to model applications using CRNS data, such as model parameter estimation and data assimilation (Baatz et al., 2017; Dimitrova-Petrova et al., 2020; Rosolem et al., 2014).

Here, we evaluate the individual impacts of relevant moderating factors on the accuracy and precision of the CRNS with two widely used analytical neutron–soil moisture interaction models, namely the NO method (Desilets et al., 2010) and the COSmic-ray Soil Moisture Interaction Code (COSMIC; Shuttleworth et al., (2013); Rosolem et al., 2014). We applied sensitivity analysis to highlight the influence of individual moderating factors on the accuracy and precision of measured neutron counts and estimated soil moisture. This sensitivity analysis provided insight on the accuracy and precision under different circumstances at our sites. That could be used to know how to improve the accuracy and how much neutron counting rates would need to be increased to obtain sufficiently precise soil moisture data. Moreover, knowing how much different factors influence the neutron count and soil moisture accuracy and precision, provides information on the data quality at different moments at a certain site and at different but comparable sites. This information is useful for both data analysis and when using the data within hydrological or land surface a modelling framework. We did this at three co-located sites in a humid region located in South England. These sites are characterized by conditions disadvantageous to the CRNS from a climatic perspective (high atmospheric pressure, high atmospheric water vapour content, often occurring intercepted water and abundant and variable biomass). Our study focuses on the following research questions:

- How do different factors affect both the accuracy and the precision of CRNS measured neutron-counting rates?
- How are those measurement quality metrics ultimately translated into soil moisture accuracy and precision?

Furthermore, note that the close proximity of the three sites allows us to investigate subtle soil and land cover related differences because the three sites essentially share the same climatological conditions, making a desired location to carry out the study.
2 | DATA AND METHODS

2.1 | Study sites

Our three study sites (named after the land cover types: grass/crop site, grass site, and shrub site) are located within a few kilometres from each other at Sheepdrove Organic Farm in South England, United Kingdom (Figure 1). The mean minimum and mean maximum temperature during the 1.5 years study period were 7 and 13°C, respectively, which compares well with the 30-year climatological record at the nearest meteorological MetOffice station in Marlborough located 22 km to the south-west (annual minimum and maximum temperatures were recorded at 5 and 14°C). The 2016 cumulative precipitation for the region encompassing the three sites was 590 mm (varying between 540 and 635 mm from site to site) which is relatively lower than the climatological record from 1980 to 2010 (815 mm a year). The time series of the measurements at the three sites are shown in Figure S1.

The soil at ‘grass/crop’ site is brown clay of about 40 cm containing flintstones and show an abrupt transition to the white chalk below. The soil cover was initially grass and later covered with spring barley eventually grazed by sheep after harvest (Table S1).

The ‘grass’ site has a grey loamy soil of about 25 cm thick containing many flints similar to the ‘grass/crop’ site. Flintstones and pieces of white chalk are more abundant throughout the soil than at the ‘grass/crop’ site and their presence increases with depth. The soil was mostly covered by grass, which was grazed by sheep and harvested. Half the field laid fallow during the final 2 months of the study period (Table S1).

The soil at the ‘shrub’ site is similar in texture to the soil at the ‘grass’ site but contains more flints which makes soil sampling more challenging here. Spatial heterogeneity in both soil texture and colour are greater at this site than at the other two sites. The vegetation is dominated by hawthorn bushes, beech trees, some cherry trees and some maple. Undergrowth (grass, clovers and other plants) was present everywhere except underneath faraway (200 m) beech trees and was present throughout the study period (varying from 20 cm high in winter to 60 cm high in summer). No substantial litter layer is present within the CRNS footprint (and therefore, while we included it in our modelling approach (Section 2.2), it does not show up in the results.

Lattice water was assumed to be 0.03 g·g⁻¹ for all three sites based on the study by Evans et al. (2016) at the same farm. Soil organic matter content (Figure S2) was determined in an aggregated soil sample per 5 cm soil layer, using the Loss on Ignition method (Hoogsteen et al., 2015). Soil organic matter was assumed to be cellulose (C₆H₁₀O₅), to have a water equivalent of 56% on mass base (Franz et al., 2013) and to be constant with time. At each site, gravimetric soil moisture samples were collected on four different days, representing a wide range of wetness conditions (Figure S3), following multiple-day calibration guidelines provided by Iwema et al. (2015) and following a standard sampling procedure (Franz et al., 2012b; Köhli et al., 2015; Schrön et al., 2017). Soil moisture content was determined with the classic oven-drying method. Undergrowth vegetation root biomass samples (three at grass/crop site, four at both grass and shrub site) were taken on the final soil moisture sampling day with a 10 x 10 cm clipper. Sample depth varied between 7 and 10 cm. Root biomass at the grass site and the shrub site were assumed constant with time, but at the grass/crop site we assumed root biomass was zero after tillage and increasing to the observed value when vegetation was present. To translate soil organic matter, gravimetric soil moisture, lattice water and plant root biomass measurements to volumetric values, dry soil bulk density was determined.
per 5 cm soil layer (0–30 cm), at four locations per site (at 2 m from the CRNS and at three locations 25 m from the CRNS; see Figure S2).

Above ground biomass was determined separately for grass/undergrowth vegetation and trees/shrubs. Grass and undergrowth biomass were sampled (7 spots at grass/crop site, 9 spots at grass site, 12 spots at shrub site) using a 25 × 25 cm clipper after measuring the vegetation height in November 2016 (biomass data from these measurements are summarized in Table S2). Wet and dry weights were obtained in a similar way as for the root biomass samples. Shrub and tree biomass at the shrub site were determined from measured tree heights and trunk circumferences at 1.5 m height. With the number of trees (from Google Earth satellite imagery) within a square of 25 × 25 m around the centre point and 25 m distance points and applying allometric relationships (above ground biomass estimates from Osbornová et al. (1990); Jenkins et al. (2003); Zianis et al. (2005) and functions from Bartelink (1997) and Forstreuter (1999) in Widlowski et al. (2003), we computed the total dry above ground tree and shrub biomass (see, for more details, the Supporting Information Section S2). We did not apply horizontal weights to the different vegetation sampling and measurement locations and locations where we determined number of trees. We computed simple means for each of our three sites.

We also used these above ground vegetation measurements to estimate leaf area index (LAI) deploying computational methods from Breuer et al. (2003) for grass and barley, from Guericke (2001) in Widlowski et al. (2003) for trees and shrubs (see, for more details, the Supporting Information Section S2). We used the LAI values (m² m⁻²) to compute vegetation interception (Pi) with the method from Von Hoyningen-Huene (1981) and Braden (1985) and obtained daily values using a 24 h moving average (see the Supporting Information Section S2). Besides soil and vegetation we took into consideration sheep grazing at the grass/crop and the grass site (Table S1) by accounting for both sheep biomass and droppings.

### 2.2 Neutron–soil moisture interaction model

We employed an extended version of the COSMIC (Rosolem et al., 2014; Shuttleworth et al., 2013). COSMIC was originally developed as a data assimilation forward operator, and is a simpler and computationally less expensive, analytical fast neutron transport model than more typical neutron particle models based on Monte Carlo approaches. The original COSMIC does not account for all neutron moderating factors relevant to our study site, including above and below ground vegetation biomass, animal biomass, organic litter layers, surface/ponding water, atmospheric water vapour, high energy neutrons intensity, atmospheric pressure and cosmic-ray sensor counting efficiency. We therefore extended COSMIC to include the effects of these factors on the computed neutron count (2). In this case, COSMIC is used to derive the equivalent neutron counts and by introducing all possible factors affecting the counting rates, the estimated neutron counts by the extended version of COSMIC \( N_{\text{p}(\text{dry})} \): the effects of atmospheric pressure \( p \), high energy neutron intensity \( I \), air humidity \( h \) and vegetation \( v \) can be directly compared with raw observed neutron counts because it includes all effects from the factors accounted for. This makes the new extended COSMIC suitable to study the effects of different natural conditions on CRNS observations through sensitivity analysis.

COSMIC considers three processes: (1) exponential moderation of high-energy neutron intensity with depth, (2) creation of fast neutrons as a consequence of collisions with soil and water particles and (3) exponential decay of fast neutrons while they travel upward from the place where they were created. These processes are captured in a single equation in COSMIC (Shuttleworth et al., 2013):

\[
N = N_{\text{COSMIC}} \int_0^{\infty} \left( \exp \left( \frac{m_w(z) - m_w(t,z)}{L_1} \right) \times \left( \frac{1}{\cos \theta} \exp \left( \frac{m_h(z) - m_h(t,z)}{L_3} \right) \right) \right) dz,
\]

where \( L_1 = 162 \text{gcm}^{-2}, L_2 = 129.1 \text{gcm}^{-2} \) and \( L_3 = 3.16 \text{gcm}^{-2} \) are universal parameter values that represent the decay of (1) high energy neutrons by dry soil, (2) high energy neutrons by water and (3) fast neutrons by water, respectively. Site-dependent parameters are \( \alpha \)—the efficiency with which fast neutrons are created, \( L_3(\text{gcm}^{-2}) \)—decay rate of fast neutrons by dry soil, and scaling parameter \( N_{\text{COSMIC}}(\text{cph}) \). Parameters \( m_w \) and \( m_h \) are the integrated mass per unit horizontal area (gcm⁻²) of dry soil and water, respectively, and \( \rho_s \) and \( \rho_w \) are the dry soil bulk density (gcm⁻³) and soil water density (here assumed to be 1 gcm⁻³). The total soil water mass includes soil moisture, lattice water (Shuttleworth et al., 2013) and soil organic matter (Baatz et al., 2014).

We made the following changes to the original COSMIC parameterization, without affecting the three key processes represented in the model:

- We used an empirical relation \( (r^2 = 0.995; \text{Iwema et al. (2015)}) \) between parameter \( L_3 \) and dry soil bulk density to derive values for \( L_3: L_3 = 106.19 \rho_s - 40.99 \).
- Whereas parameter \( \alpha \) has been assumed site dependent in the past, in this study we fixed it at 0.2 after preliminary results showed that at all three Sheepdrove sites and three other sites (Santa Rita Creosote in the USA and Rollesbroich and Wuestebach in Germany; Franz et al., 2012a; Baatz et al., 2014; Iwema et al., 2015) this parameter converged to values around 0.2.
- \( L_3 \) varies with depth, as a function of the vertically varying dry soil bulk density and below ground hydrogen pools.
- In addition, we added dry root biomass and defined both this new hydrogen pool and soil organic matter as dry biomass (g) per cubic centimetre of soil and assumed dry biomass is cellulose (Franz et al., 2013). Within the model, the water equivalents are calculated for each of these separate hydrogen pools and are then added up to a single water equivalent per soil layer.
Ponding water, litter layer and animal droppings were represented by individual 0.1 cm surface water equivalent layers that can be added up depending on the amount of surface water equivalent. Whereas these different hydrogen pools can be added as different inputs to the model, within the model they are summed to a single water equivalent.

To determine the naturally occurring neutron count with the extended COSMIC, we added the effects from the equivalent water of above ground biomass, intercepted water and sheep biomass to the COSMIC modelled neutron counts following the function developed for above ground biomass by Baatz et al. (2015). Within the model, this function is applied to the summed water equivalent.

Similarly, we added the effects of atmospheric water vapour using the approach by Rosolem et al. (2014).

We also added the effects of the atmospheric pressure (Bogena et al., 2013; Zreda et al., 2012), and temporal changes in high-energy neutron intensity (Zreda et al., 2012).

The final neutron count containing all the effects from these factors, above ground biomass, surface and soil is denoted \( N_{\text{pihv}} \) (Figure 2).

### 2.3 Calibration strategy and sensitivity analysis

In this study, we investigate the accuracy and precision of both neutron count and soil moisture estimate separately. We quantify the accuracy of the neutron count (cph) and the soil moisture (cm\(^3\) cm\(^{-3}\)) estimate as the change in the number/quantity as a result of a change in input values. The neutron count precision has a Gaussian distribution at counts above 30 cph and can then be defined as the square root of the measured neutron count (Knoll, 2000; Zreda et al., 2012):

\[
\sigma_N = \sqrt{N}
\]  

Usually however, the neutron count precision is defined as a more informative, relative precision, by dividing \( \sigma_N \) over the neutron count itself, obtaining the coefficient of variation (CV):

\[
CV = \frac{\sigma_N}{N}
\]

As a first step to assess the neutron count accuracy, we calibrated parameter \( N_{\text{COSMIC}} \) of both the original and extended COSMIC with data from three (grass/crop site) to four (grass and shrub sites) sampling days. By comparing the multi-day calibrated soil moisture-neutron count curves of the three different sites for both COSMIC versions, we gained a first insight of the effects of the different time variant neutron moderating factors. We generated a sample of 1450 values for parameter \( N_{\text{COSMIC}} \), evenly spaced at an interval of 0.5 cph. To compute CRNS-footprint average soil moisture values we used the horizontal and vertical weighting formula’s from Köhli et al. (2015) and Schrön et al. (2017).

To investigate the neutron count accuracy and both neutron count and soil moisture precision more thoroughly, we employed sensitivity analysis. We used the global sensitivity analysis algorithm PAWN (Pianosi & Wagener, 2015) within the SAFE Toolbox (Pianosi et al., 2015). PAWN computes cumulative density functions and therefore works for any output distribution (for instance non-Gaussian distributions). The algorithm uses a so-called unconditional sample and multiple so-called conditional samples. An unconditional (Latin Hypercube) sample is constructed by varying all input variables within defined ranges. Thereby the output variation as a result of the total variation of all input variables. The conditional samples are constructed by varying all but one input within their ranges. The difference between the output variation of the unconditional samples and a conditional sample carries information about the effect of the input variables.

![FIGURE 2 Model structure with input and output for the original (bold, italic text) and the extended COSMIC (plain text). In this case, \( N_i \) is the simulated neutron count with added effects from soil and surface hydrogen pools and can be compared with measured neutron counts corrected for above ground effects. \( N_v \) also carries the effects from above ground biomass. \( N_{\text{pihv}} \) carries the effects from all factors and can therefore be compared with uncorrected, measured neutron counts.](image-url)
that was fixed to make the conditional sample. PAWN computes sensitivity indices for which a higher value indicates a greater influence on the model output.

We designed four synthetic experiments using PAWN at each of our three sites. The first experiment (S1) was to compare the effects of neutron-moderating factors and to see how much uncertainty in dry soil bulk density samples can affect the neutron count. The other three experiments (S2–S3) provided insight about how the hydrogen pools other than soil moisture affected the outputs at dry (0.1 cm$^3$ cm$^{-3}$), average (0.3 cm$^3$ cm$^{-3}$) and (0.6 cm$^3$ cm$^{-3}$) soil conditions, respectively. In the first experiment, 13 model inputs were varied, whereas in the other three experiments soil moisture was fixed and therefore 12 inputs were varied.

We determined the site-specific upper bounds of the input ranges (Table 1) from the maximum estimated values obtained from in situ samples. The minimum values for all variables were set to zero, except for dry soil bulk density, atmospheric pressure and the high-energy neutron correction factor, which were set according to observed minimum values measured in the field. We assumed the mean observed values minus plus the standard deviations from our measurements for the dry soil bulk density minima and maxima, respectively, and rounded to the lower and higher first digit, respectively. In the sensitivity analysis we change the values of the soil properties (soil bulk density, lattice water, soil organic matter, and root biomass values) by a percentage based on the upper 5 cm value and its absolute error (determined by samples in the lab). The rest of the profile is changed relatively to these values. This avoids negative values and allows to vary just one value per variable with each sensitivity run, rather than varying the value of each layer separately. To establish the maximum values for soil moisture content, we used both the footprint average soil moisture contents from the soil samples and the point-scale soil moisture observations. We used homogeneous soil moisture profiles only, because the focus of this study was on the contribution of the integrated water content from the sensor, regardless of profile characteristics, which simplifies the design of our sensitivity analysis experiments substantially.

We used a sample size of 1500 model runs for the unconditional sample and a sample size of 1000 runs for each conditional sample. For each variable 10 different conditional samples were used to obtain statistically robust results. Namely, a single conditional sample per parameter carries a too great risk of yielding a biased and thereby insufficiently representative representation of the parameter’s space.

### Table 1: PAWN sensitivity analysis input ranges

| Input       | Unit          | Min. (all sites) | Max. grass/crop site | Max. grass site | Max. shrub site |
|-------------|---------------|------------------|-----------------------|-----------------|-----------------|
| sm          | cm$^3$ cm$^{-3}$ | 0.0              | 0.6                   | 0.6             | 0.6             |
| bd (top layer) | g cm$^{-3}$   | 1.0/0.9/0.7      | 1.6                   | 1.1             | 1.0             |
| lw (top layer) | g cm$^{-3}$   | 0.05             | 0.04                  | 0.03            |                 |
| so (top layer) | g cm$^{-3}$   | 0.12             | 0.14                  | 0.14            |                 |
| ro (top layer) | g cm$^{-3}$   | 0.002            | 0.010                 | 0.031           |                 |
| dr          | kg m$^{-2}$   | 0.02             | 0.02                  | 0.00            |                 |
| po          | kg m$^{-2}$   | 5.0              | 5.0                   | 0.0             |                 |
| ag          | kg m$^{-2}$   | 0.7              | 1.7                   | 3.3             |                 |
| pi          | kg m$^{-2}$   | 2.6              | 2.5                   | 2.3             |                 |
| a           | kg m$^{-2}$   | 0.08             | 0.07                  | 0.0             |                 |
| ah          | gm$^{-3}$     | 17.6             | 17.6                  | 17.6            |                 |
| p           | hPa           | 940              | 1030                  | 1030            | 1030            |
| fi          | –             | 0.9              | 1.1                   | 1.1             | 1.1             |

Note: Dry soil bulk density had different minimum values for the three sites, indicated with the dashes. The minimum values for the hydrogen pools were set at zero, so that the effect of the magnitude of these variables on the accuracy and precision could be determined. The minimum values for dry soil bulk density, atmospheric pressure and incoming neutron intensity were set to minimum observed values, rounded to the lowest significant decimal or integer. The maximum values for all input variables were determined from observations at the three sites and rounded to the highest significant decimal or integer. The soil moisture maximum was set to the (rounded) maximum value observed in soil sample, fixed and mobile device point scale soil moisture sensors data used. The maximum values for lattice water, soil organic matter, plant roots and above ground biomass, were set at the observed means plus one standard deviation. The sheep dropping maximum value was estimated from the mass and water content observed in sheep droppings combined with a field estimate of density on the fields concerned. Ponding water was based on the water depth observed during one ponding event. The maximum intercepted water value was based on the maximum value computed from the combination of precipitation and vegetation LAI, applying the functions from Von Hoyningen-Huene (1981) and Braden (1985). The maximum values for atmospheric humidity, atmospheric pressure and incoming neutron intensity were based on the maximum observed values of the three sites combined, using the CRNS temperature, humidity and pressure sensors. The maximum value of the incoming neutron intensity was taken from the maximum value from Jungfraujoch. Abbreviations: a, sheep biomass; ag, above ground vegetation dry biomass; ah, absolute atmospheric water vapour content; bd, bulk density; dr, sheep droppings dry biomass; fi, high-energy neutron intensity correction factor; lw, lattice water; p, atmospheric pressure; pi, intercepted water; po, ponding water; ro, dry root biomass; sm, soil moisture; so, soil organic matter.
The total number of model evaluations per PAWN experiment was therefore $1500 + 1000 \times 10$ conditional samples $\times 14$ variables $= 141500$ of our maximum number of variable inputs of 14.

The number of 14 variables stems from using 13 model variables and 1 dummy factor in the sensitivity analyses. This dummy factor did not affect the model output and could therefore be used to establish a threshold value for each experiment, below which sensitivity index values for the other (real) factors were considered negligible (Zadeh et al., 2017). The threshold value was the upper bound of the uncertainty range of the dummy’s sensitivity index, established from bootstrapping. Bootstrapping means taking subsamples and helps identify if the variation within the main sample was sufficiently small, or in other words that the main sample was sufficiently large.

The soil moisture precision is a function of the coefficient of variation (which is a function of the uncorrected measured neutron count) and the neutron count corrected for factors other than soil moisture. While the extended COSMIC can compute neutron counts from soil moisture profiles and other neutron moderating factors, it does not directly allow for the computation of soil moisture precision. To obtain soil moisture precision values, we combined the extended COSMIC and the Desilets function (Bogena et al., 2013; Desilets et al., 2010; Schrön et al., 2017) within a framework, as depicted in Figure 3. We increased the offset in this formula by accounting for plant root, biomass, ponding water and animal droppings, yielding an extended $N_0$ function:

$$
\theta = \frac{0.0808 \rho_s}{N_0} - 0.372 \cdot \frac{\rho_s}{\rho_s} - l_w - w_{\text{SOM}} - w_{\text{roots}} - w_{\text{pond}} - w_{\text{droppings}},
$$

where the parameter values $a_0 = 0.0808 \text{cm}^3 \text{g}^{-1}$, $a_1 = 0.372 (-), a_2 = 0.115 \text{cm}^3 \text{g}^{-1}$ and $N_0 (\text{cph})$ is a site dependent normalization parameter. Parameters $l_w$ and $w_{\text{SOM}}$ are the CRNS-footprint average volumetric lattice water content and soil organic matter equivalent water content ($\text{cm}^3 \text{cm}^{-3}$), respectively, and $\rho_s \text{(g cm}^{-3}\text{)}$ is the dry soil bulk density, usually determined from soil samples. $N$ is the measured neutron count, usually corrected for neutron mitigating factors (e.g., $N_{\text{phv}}$) $\theta$ is CRNS-footprint average volumetric soil moisture content ($\text{cm}^3 \text{water cm}^{-3} \text{soil}$). The newly added parameters are: $w_{\text{roots}}$ is the plant root water equivalent, $w_{\text{pond}}$ is the ponding water and $w_{\text{droppings}}$ is the animal droppings water equivalent, all in volumetric water content. We combine the neutron counts obtained with the extended COSMIC and the $N_0$ method, resulting in two estimates of soil moisture. The difference between these two values divided by two gives an estimate of the precision. We remark that this quantity is technically not a standard deviation. Due to the non-linear conversion function, $\theta(N, N_0)$, the error in soil moisture is asymmetric. For a symmetrical approximation of the propagated uncertainty, the reader is referred to Jakobi et al. (2020).

The $N_0$ method contains some simplifications compared to the extended COSMIC (e.g., the water equivalent of ponding water, animal droppings, lattice water and organic litter layer was defined as a water layer within the soil), which cause minor differences in the shapes of both calibration curves.

### 3 | RESULTS

#### 3.1 | Accuracy

We first investigated the neutron count and soil moisture estimate accuracy through calibrating both the original and the extended COSMIC at all three sites and with data from the different calibration days. The results from these analyses provide insight into the effects of different local hydrogen pools that have traditionally not always been accounted for (e.g. vegetation, intercepted water, plant roots and animal droppings) when using cosmic-ray neutron data. Figure 4 shows the multi-day calibration curves of both the original (left panel) and extended (right panel) COSMIC, at all three sites (grouped together in

**FIGURE 3** Flowchart of the method used to compute soil moisture precision as employed within the PAWN sensitivity analysis experiments. $N_{\text{phv}}$ is the neutron count computed by the extended COSMIC which contains the effects of all factors accounted for and which can be compared to measured, uncorrected neutron counts. $N_{\text{soil}}$ is the COSMIC neutron count which contains the effects from all hydrogen pools within the soil and which are simulated as a layer on top of the soil (ponding water, litter layer and animal droppings). $\sigma_N$ is the standard deviation on $N_{\text{soil}}$. 


Multi-day COSMIC calibration curves for the three sites. The left plot shows the calibration curves when taking into consideration only more commonly measured neutron-moderating factors (lattice water, soil organic matter, dry soil bulk density, atmospheric water vapour, atmospheric pressure, high-energy neutron intensity). The right plot shows the calibration curves taken into account, besides the before-mentioned factors, the additional hydrogen pools (above ground vegetation biomass, plant roots and animal droppings) with the extended COSMIC. The neutron counts in the right plot are corrected for above ground biomass and vegetation intercepted water. The markers indicate the calibration points.

The visibly greatest difference is for the shrub site curve, where the difference for the original COSMIC is 70 cph (5% of the 1450 cph neutron count) and for the extended COSMIC it is 30 cph (2% of the 1450 cph neutron count). The calibrated parameter for the extended COSMIC was 613 cph. Thereby the calibration curve of the extended COSMIC at the shrub site was closer to the curves of the other two sites than to the original COSMIC curve of the shrub site. The changed curve position corresponds with differences between the original COSMIC curve and the extended COSMIC curve in soil moisture estimates of up to 0.07 cm<sup>3</sup> cm<sup>-3</sup>, at a 0.6 cm<sup>3</sup> cm<sup>-3</sup> soil moisture content. These effects on both neutron count and soil moisture accuracy can be attributed to the relatively great abundance of above ground biomass, whereas intercepted water and plant root biomass had little effect.

We investigated that by running additional calibrations (curves not shown) in which we included only (1) above ground biomass and (2) above ground biomass and intercepted water. Whereas the calibrated parameter for the original COSMIC was 586 cph for COSMIC without additional hydrogen pools (left panel of Figure 4), it was 605 cph with above ground vegetation biomass, 607 cph with both above ground biomass and intercepted water, and 613 cph when all additional hydrogen pools were included (right panel of Figure 4). This result shows above ground biomass had the greatest effect of not regularly measured hydrogen pools on the accuracy. This is not a surprising result given the water equivalents of other not regularly accounted hydrogen pools are clearly smaller at these sites.

3.2 | Precision

Figure 5 shows the results for the neutron count precision (CV). The neutron count precision (CV) is directly related to the neutron count accuracy (a change in neutron count due to a change in the magnitude of a certain neutron moderating factor), through multiplication with the neutron count. Therefore, the neutron count precision sensitivity analysis also provides information on the neutron count accuracy. Therefore, in this section we mention the neutron count accuracy as well. The upper panel of Figure 5 shows the sensitivity analysis results for the first experiment, for which all relevant factors were varied (see Figure S4 for a plot zoomed in on the least influential input variables). We compare the sensitivity indices with a defined threshold obtained with a dummy parameter. If the sensitivity index lies below this threshold, the effects are regarded as insignificant. Site-to-site differences appear to be small. At all three sites atmospheric pressure and soil moisture content were, respectively, more than seven and four times more influential than the other factors. The only other factors that were significantly influential at all three sites were dry soil bulk density, high-energy neutron intensity and atmospheric water vapour. Soil organic matter and ponding water exceeded the threshold at least at one site. The maximum ponding water layer (5 cm) was however a rough estimate and ponding water rarely occurred and in any case lasted for a few consecutive hours only. Despite the substantial effects of above ground biomass on the CRNS calibration results compared to other not regularly measured neutron moderating factors, the relative influence of above ground biomass this factor on neutron count accuracy and precision was substantially lower compared to the more regularly determined soil bulk density, lattice water and soil organic matter, with 50%–100%, 20%, and 40%, respectively. These results overall indicate that at our three sites the neutron moderating factors traditionally accounted for (bulk density, lattice water, soil organic matter, atmospheric water vapour, atmospheric pressure and high-energy neutron intensity) have substantially greater influence on neutron count accuracy and precision than factors that are taken into account less often, like above ground vegetation biomass.

Next, we look at the other three sensitivity experiments, in which the effects of neutron moderating factors at three different soil moisture levels, on neutron count accuracy and precision were investigated (grass/crop site shown in the lower panel of Figure 5; between-site differences were small). Differences in sensitivity to the different factors (excluding wetness level) between the three wetness levels are visibly small. Compared to wet soil state, at dry soil state the influence of atmospheric pressure was 10% smaller. Oppositely, the influence of dry soil bulk density, lattice water and soil organic matter was...
20%–80% larger at the dry soil state than for wet soil. These effects can be explained from the non-linear shape of the neutron–soil moisture relationship. Under dry soil conditions, a small difference in soil water equivalent (e.g., soil moisture or lattice water) or dry soil bulk density yields a relatively large difference in neutron count, whereas for wet soil the opposite is true. The sensitivity analysis results indicate that time-variable and not regularly quantified hydrogen pools, like biomass, affect the neutron count accuracy and precision less than regularly quantified factors (like atmospheric pressure and high-energy neutron intensity) and are, according to the threshold definition, insignificant. The calibration results however showed that the effects from these hydrogen pools on the accuracy of the soil moisture estimate are substantial.

We now look at the sensitivity analysis results of the soil moisture precision. The results for the first experiment (all factors variable; upper panel of Figure 6, see Figure S4 for a plot zoomed in on the least influential input variables) show that, in contrast with the results for the neutron count accuracy and precision, the soil moisture precision is largely (minimum 10 times more) a factor of soil wetness compared to other factors. This means that although different factors are important to neutron count accuracy and precision, they are not as important to soil moisture precision. The only other three factors that were above the threshold at least for one site were atmospheric...
pressure, dry soil bulk density and soil organic matter. The explanation for the large effect of soil moisture content on the precision of the soil moisture estimate is the non-linear shape of the negative hydrogen pools–neutron count relationship. Factors (like atmospheric pressure) that were shown to have a strong effect on neutron count accuracy and precision and on soil moisture accuracy, had less effect on soil moisture precision. The reason is that a difference in neutron count causes a shift in the location of the calibration graph, but the slope of the curve changes much less considerably.

When we look at the lower plot of Figure 6, we see that considerable differences between wetness levels exist for soil moisture precision. At dry conditions lattice water and soil organic matter are 30%–120% more influential than at medium or wet conditions, whereas during wet conditions the dry soil bulk density is 100%–300% more influential than at the other wetness conditions and the atmospheric pressure is the most influential factor (80%–150% more influential than dry soil bulk density). At dry conditions the water equivalents are relatively large compared to other hydrogen pools, including soil moisture content, which is affected by the dry soil bulk density parameter. The greater influence of atmospheric pressure at wet conditions is a combination of the smaller influence of the other factors (so the influence of atmospheric pressure increases relatively) and to some extent of direct effects on neutron count. Like the previous experiments, this analysis shows limited effects of less commonly measured neutron counts on the sensitivity.

Finally, to obtain sufficiently precise soil moisture estimates, it is important to know the expected magnitudes of the soil moisture precision. We therefore computed the best (minimum) and worst (maximum) soil moisture precision values from the three sensitivity analysis experiments that represented the three different wetness levels (0.1 cm$^3$ cm$^{-3}$, 0.3 cm$^3$ cm$^{-3}$ and 0.6 cm$^3$ cm$^{-3}$). Under driest conditions (0.1 cm$^3$ cm$^{-3}$), a 1 h neutron count integration time yielded a best case (minimum) precision of 0.01 cm$^3$ cm$^{-3}$ and a worst case (maximum) precision of 0.02 cm$^3$ cm$^{-3}$. However, under the wettest soil conditions the best precision was 0.06 cm$^3$ cm$^{-3}$ and a worst precision was 0.13 cm$^3$ cm$^{-3}$. Differences between sites were in all cases, except for the maximum precision values, below 0.01 cm$^3$ cm$^{-3}$. Under wet conditions, the maximum precision value at the shrub site was just over 0.01 cm$^3$ cm$^{-3}$ higher than the corresponding value at the grass/crop site.

To obtain a sufficiently low precision value, the neutron count integration time can be increased. Comparing precision values with those of other soil moisture sensors can provide an idea of how good they are. We compared against typical precision values of Soil Moisture Ocean Salinity satellite (SMOS; Kerr et al., 2001) and TDT (0.02 cm$^3$ cm$^{-3}$; Topp et al., 2001)) to investigate which integration time lengths would be needed to obtain sufficiently low precision values. To this purpose, we computed the soil moisture precision not only for a 1 h integration time, but for every hour up to 48 h integration time (Table 2). At dry conditions 2 h integration time would suffice to achieve TDT precision, whereas under wet conditions a 40 h integration time would be needed (consistent with Bogena et al. (2013)). Additional analysis with point-scale soil moisture as input showed that during the study period a 4 h integration time would always have sufficed to meet SMOS precision (data not shown). To meet TDT precision a 14 h integration time would always have been enough. The reason is that the profile average soil moisture content never reached values above 0.5 cm$^3$ cm$^{-3}$.

### Table 2

| Climate | Average $\theta$ | Precision ≤ 0.04 | Precision ≤ 0.02 |
|---------|-----------------|------------------|------------------|
| Dry     | 0.1 cm$^3$ cm$^{-3}$ | 1 h               | 2 h               |
| Average | 0.3 cm$^3$ cm$^{-3}$ | 2 h               | 7 h               |
| Wet     | 0.6 cm$^3$ cm$^{-3}$ | 11 h              | 40 h              |

Note: Values shown were obtained from PAWN sensitivity analyses for the shrub site. The values at the two other sites were equal or slightly lower.

## 4 | DISCUSSION

Assessing the uncertainty of measured cosmic-ray neutrons and consequently the estimated soil moisture is of particular importance especially in more humid regions (Bogena et al., 2013), like in South England, where observational uncertainties are expected to be relatively high and more difficult to be quantify. Our results complement recent findings about the accuracy and precision of CRNS soil moisture data (Baroni et al., 2018; Gugerli et al., 2019; Jakobi et al., 2020; Weimar et al., 2020).

The work by Baroni et al. (2018) presented uncertainty analysis and sensitivity analysis on different neutron mitigating factors at two sites in Germany. The major methodological difference between their and our studies is that Baroni et al. analysed the uncertainty on the entire time series, applying standard deviation and root mean squared error (RMSE), while we separated accuracy and precision looking at individual neutron count integration time steps. Comparing our accuracy and precision values to their RMSE and sensitivity values is therefore not sensible. With regards to the results, the authors found that the soil moisture estimate was particularly sensitive to the vertical variability in the soil moisture profile, to dry soil bulk density, and to incoming neutron variation. While we did not explicitly take vertical soil moisture variation into account, our study confirmed that soil moisture precision is most sensitive to the soil moisture content itself. We further unravelled the influence of dry soil bulk density, incoming neutron correction and many other factors on the neutron count accuracy and precision, and on the soil moisture precision. On the other hand, we found atmospheric pressure to be influential on accuracy and precision of both, neutron counts and soil moisture, which was not considered by Baroni et al.

In general terms, our study aimed at completing the picture of all neutron-mitigating factors involved.
The role of above ground biomass provides further insight to presented results. We found that vegetation is not influential within our sensitivity analysis, but in contrast, it substantially affected the final soil moisture product when it is not corrected for. Baroni et al. (2018) did not find evidence for such an effect, which demonstrates that the derived level of sensitivity is often highly specific to sites, methods and the objective of the study. The use of observational values that are typical for humid climates also comes with limited transferability of the results to very rare and extreme climates. For example, dynamics of atmospheric water vapour are typically much less influential than soil moisture, but a recent study by Köhli et al. (2021) has demonstrated that it can become the dominating factor for CRNS accuracy in arid regions ($\theta \approx 0.05 \text{cm}^3/\text{cm}^2$).

The time variable spatial effects of animals could be hardest to quantify. However, we expect this factor to be of limited relevance at most sites, because the periods in which the animals would gather near the sensors were usually short-lived. Besides the fact that we found low sensitivity to this factor in our analysis. This type of potential source of uncertainty does however indicate that it is important to combine modelling and sensitivity analysis with field knowledge. Making assumptions on spatial distributions (e.g., a spatially uniform distribution of vegetation and animals), rather than modelling them all in great detail, would require much more computationally demanding calculations, with a model like URANOS (Köhli et al., 2015). The purpose of our approach, employing an extended COSMIC model, is however to make sensitivity analysis, site-specific features and dedicated modelling quicker to implement.

Notice that we chose not to account for possible additional sources of uncertainty introduced by the technique of soil sampling, such as gravimetrically determined soil moisture content, the limited number of samples used for estimating dry soil bulk density, limited number of vegetation samples and uncertainties related specifically to our allometric calculations for vegetation biomass. Such sources of uncertainty are partly due to spatial distribution of different hydrogen pools within the CRNS footprint, which can vary over time. These effects can be greater at sites with larger spatial variability, as is the case at our sites for soil conditions, due to the abundance of stones, and for vegetation biomass, at both the shrub site (great spatial heterogeneity) and grass and grass/crop sites (spatial and temporal heterogeneity). This effect is greater when spatial heterogeneity is larger, both vertically and horizontally. The CRNS footprint changes over time (Köhli et al., 2015), and both horizontally (~10m) and vertically (~10cm) this can lead to some decreased match with the sampling scheme (see, e.g., Schrön et al., 2017). At our three sites the vertical CRNS penetration depth was however estimated not too exceed the sampling depth of 30 cm. Therefore, we expect this issue to be of limited relevance at our specific sites.

Uncertainties in the sampling techniques are somewhat universal to soil moisture measurements, techniques, and our focus in this study has been on highlighting the uncertainties related specifically to the nature of the CRNSs and their response to the environment. The approach we used for field sampling follows general guidelines adopted by the wider CRNS community regarding sampling designs (Franz et al., 2012b; Iwema et al., 2015; Schrön et al., 2017). Despite the limitation originating from limited sampling, by using feasible site-specific ranges based on actual measurements, our approach provided a thorough first insight adopting a more realistic variation of neutron mitigating factors (as opposed to randomly varying such factors). Even when all neutron-moderating factors deemed relevant are taken into consideration at a CRNS site, some residual variability in measured neutron counts will remain. This is expected and due to insufficient measurement precision.

The definition of stochastic uncertainty we used in this paper is based on a direct calculation ($\theta/N \pm d\theta/N$, Figure 3). Previous studies applied approximations on the first order (Gugler et al., 2019; Weimar et al., 2020) or third order of Gaussian error propagation (Jakobi et al., 2020), which would lead to less accurate results especially in cases of extreme soil moisture ranges. On the other hand, our final estimation of the soil moisture precision is limited due to combining the extended COSMIC with the extended N0-method. In the sensitivity analysis, we used vertically constant soil moisture contents and therefore the lack of vertical heterogeneity in the N0-method would not be expected to affect the soil moisture precision values considerably. Nevertheless, all of these methods are approximations of a completely exact solution, albeit for different reasons.

The available detector-specific stochastic uncertainty directly determines the lower bound of the recommended temporal aggregation period. We found that at our sites, in order to achieve soil moisture precision comparable to typical TDT products (0.02 cm$^3$ cm$^{-3}$), CRNS data should be integrated between 2 h (dry soil moisture conditions; 0.1 cm$^3$ cm$^{-3}$) and 40 h (wet soil moisture conditions; 0.6 cm$^3$ cm$^{-3}$). During most of the study period however, a time length of a day or less would probably have sufficed, corresponding to currently common standards of neutron count integration times. This is true at least for our site and possibly for sites with similar high organic matter content, high atmospheric humidity, similar biomass and intercepted water. In fact, at sites with lower abundance of these additional hydrogen pools the needed integration times would be even lower. We note that the integration time lengths mentioned in the results section, are likely valid only for the detector used in this study. Nevertheless, our findings can provide a reference also for other sensor types when the relative difference of the count rate is taken into account. The proper determination of integration periods is relevant when using the CRNS data for a specific purpose, like studying the effects of storm rainfall or irrigation on soil moisture content. Such effects, which develop over a relatively short time in the order of hours, could possibly not be studied with sufficiently good soil moisture estimate precision. In these situations, the precision could be improved towards a satisfactory level by, for instance, more efficient detectors (Weimar et al., 2020), larger instruments (Jakobi et al., 2020) or a combination of sensors (Fersch et al., 2020; Schrön et al., 2018).

5 | CONCLUSIONS

We separately investigated the accuracy and precision of the CRNS at three sites located within a few kilometres from each other in South
England. CRNS accuracy and precision are two distinct metrics and can be improved only separately. Whereas the accuracy can be improved by correcting for neutron moderating factors other than soil moisture, the precision can be improved by increasing the neutron counts within a certain time interval.

All factors however influence, to various extends, the accuracy and precision of the measured neutron counts and the soil moisture products derived from them, in different ways. Knowing which factors are more influential on both quality metrics provides improved insight in the data quality. We therefore investigated the effects of different relevant neutron-moderating factors on both the CRNS neutron count accuracy and precision and on the CRNS soil moisture estimate accuracy and precision. Hydrogen pools like soil moisture and the measured epithermal-fast neutron count have a non-linear relationship that makes these two quantities have different dependencies on different neutron moderating factors. To this purpose we extended the COSMIC, which included relevant neutron moderating factors. We employed both calibration and sensitivity analysis with the extended COSMIC, to separately investigate accuracy and precision.

The sensitivity analysis and calibrations showed that atmospheric pressure and soil moisture content affected neutron count accuracy most. These two factors were, respectively, seven and four times more influential than the other factors. Despite having considerably less effect on neutron count accuracy than regularly measured factors (e.g., atmospheric pressure, soil organic matter), less regularly measured, time-variable hydrogen pools like above ground biomass substantially affected the accuracy of the soil moisture estimate. The differences amounted up to \(0.07 \text{ cm}^2 \text{ cm}^{-3}\) and implied that if these time-variable hydrogen pools were not accounted for during calibration, considerably inaccurate soil moisture estimates could result. The mentioned soil moisture estimate differences equate to dry above ground biomass differences of up to \(\sim 3 \text{ kg m}^{-2}\). Due to the mathematical relationship between neutron count and its relative precision (coefficient of variation), the dependency of neutron count accuracy and precision on different neutron moderating factors is the same. However, this is not true for the precision of the soil moisture estimate, due to the non-linear, inverse relationship between neutron count and hydrogen pool density. The precision of the CRNS soil moisture estimate was mostly a function of the soil moisture content itself. The second most influential factor, atmospheric pressure, was 10 times less influential. Not regularly measured hydrogen pools like above ground biomass and vegetation intercepted water thereby had little effect on CRNS soil moisture precision at our sites.

To obtain sufficiently accurate CRNS soil moisture estimates, we recommend to determine all relevant hydrogen pools (see also Baroni & Oswald, 2015) on calibration days and preferably estimate them for the entire time series, such as above and below ground biomass and vegetation intercepted water. Temporally stable variables need to be determined only once. We found that at our sites an integration time length of a day or less would suffice, corresponding to currently common neutron count integration times. The integration time values from our sites cannot be directly transferred to other sites, but are indicative for sites with similar high organic matter content, high atmospheric humidity, similar biomass and intercepted water. To estimate CRNS precision, required integration time and the effects of different neutron-moderating factors on CRNS accuracy at other humid sites in the UK and beyond, the extended COSMIC can be used in combination with calibration and sensitivity analysis. Hydrogen pools not included within this study, like snow (which was never present at our sites), can be easily included within the extended COSMIC.

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**CONFLICT OF INTEREST**

We foresee no conflicts of interest.

**DATA AVAILABILITY STATEMENT**

The data collected from our three sites at the Sheepdrove Farm is available at the Natural Environment Research Council’s Data Repository for Atmospheric Science and Earth Observation Archive (CEDA) [https://catalogue.ceda.ac.uk/uuid/cef0068506d0458f903bd79edbf9df31].

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