# Response to Interactive comment by H. Bogena (Referee)

Comments from referee are printed in black. Authors' responses are printed in red.

I have reviewed this manuscript for the second time. The authors have improved their manuscript considering most of my earlier comments. It will be a nice contribution to the HESS. However, there are still several minor issues which need to be considered: We would like to thank this reviewer for assessing our manuscript for a second time. We were fortunate to have three reviewers that took their job seriously and genuinely cared about the quality of the work and the subject matter.

As mentioned in my earlier review, calibration has to be performed using the total hydrogen pool, and soil moisture is then computed by subtracting other hydrogen pools than soil moisture from the measured neutron-derived soil moisture. Also the authors have stated in their cover letter that this procedure was applied in this study but this procedure is still not clearly stated in the revised manuscript and it is also not mentioned in their "Best practice" description.

Thank you for reminding us of this missing piece of information. We added in line 231: 'Calibration has to be performed using the total belowground hydrogen pool (including hydrogen contributions from lattice water (WL), soil organic matter (SOM) and root biomass (BR)). Soil water content is then computed by subtracting the other hydrogen pools from the measured neutron-derived signal.'

In my first review I have stated the following: "The results plotted in Fig. 12 show clearly, that only the most extreme dry and wet samplings result in an acceptable calibration result, whereas sampling at intermediate soil moisture will lead to very uncertain calibration of the modified N0-method. On the other hand, this illustrates the value of the standard N0-method that will also produce stable results in case only one sampling date is available. Please add this to the discussion."

The authors answer was: "Fig. 9 shows that the best 2-point-calibrations are achieved with one sampling point taken under very dry conditions and another sampling point taken either under intermediate or wet conditions. In our case it is hard to see the value of the standard N0-method since it always resulted in too much soil moisture variability no matter whether the calibration was performed during wet, intermediate or dry conditions (because the standard calibration of N0 does not allow a change of the slope of the calibration function)."

Clearly the authors didn't fully grasp my comment. The value of the standard N0-method lies in its predefined form that makes calibration using data from a single sampling date more stable than the modified N0-method. This should be added to the discussion since there might be cases where only one calibration date is available.

Ok, we acknowledge the fact that the standard N0 method does have its value when using only a single calibration. We added in line 587 of the discussion: 'The value of the

standard N0-calibration method becomes apparent when there is only data available from one calibration date. Due to the fixed shape of its calibration function, the general dynamics of the soil water content will still be reproduced.'

L47: ...neutrons interact with air and soil nuclei... Done.

L414: delete "resolution" Deleted.

Figure 1: The blue dots are difficult to discern. We turned them into white dots.

Figure 2: The modified schematic shown in this figure is still confusing. Why should the factors influencing the cosmic-ray intensity a ground level be symbolized a rays of different length? I find this irritating and not helpful for the understanding of the involved processes. In addition, the presented sensing depth boundaries are too numerous be discernible and the distribution is not correct. A better representation can be found in Köhli et al., 2015. Thus, in my opinion the figure should be omitted.

We modified the figure to address your concerns. We removed the rays of different length and instead used gradually less intense background color to represent the decreasing number of fast neutrons due to the various factors. We removed all depth boundaries only keeping the maximum extent and one example of reduced depth and footprint. We also modified the shape of the depth boundary so that it resembles better what Köhli et al. (2015) describe.

# Response to Interactive comment by Anonymous Referee #2

Comments from referee are printed in black. Authors' responses are printed in red.

The authors have addressed my comments and concerns.

We would like to thank this reviewer for assessing our manuscript for a second time. We were fortunate to have three reviewers that took their job seriously and genuinely cared about the quality of the work and the subject matter.

# Response to Interactive comment by Anonymous Referee #3

Comments from referee are printed in black. Authors' responses are printed in red.

This paper describes experimental work whose goal was to calibrate cosmic-ray soil moisture probe used in the presence of variable vegetation. I have reviewed this paper before and recommended it to be published with minor revisions. This second submission is much improved. My recommendations, as well as those of other reviewers, have been taken seriously and the improved manuscript is very good. I recommend that it be published, subject to minor technical revisions as described in the attached annotated manuscript.

We would like to thank this reviewer for assessing our manuscript for a second time. We were fortunate to have three reviewers that took their job seriously and genuinely cared about the quality of the work and the subject matter.

L16: give max deviation in absolute values and also as % of the total range Added: '...deviations of up to 0.1 m<sup>3</sup> m<sup>-3</sup> (24 % of the total range)...'.

L20: change to "correctly to define"

Changed to: 'A two-point calibration was found to effectively define the shape of the modified calibration function...'.

L48: "fast neutrons" means specific energy (around 1 MeV), so there is no need to qualify this. Removed.

L603: this is not a calibration method, but a model of neutron intensity that can be used in data assimilation schemes - please clarify this in text.

Changed to: '...another parameterization method developed by Shuttleworth et al. (2013) (the COSMIC operator, a model of neutron intensity used in data assimilation schemes)...'

L660: I am not sure if this is best practice. It is yours, but to be best it should be confirmed by others. I suggest deleting this appendix. Or, at the very least, present it as a proposal for consideration by users.

You are right in that we should not call it 'best practice'. This would indeed be overconfident. Therefore we changed the name to 'Proposed method for calibration...' We would, however, like to keep the Appendix in the manuscript since it provides the sequence of necessary steps that first-time users can follow when they set up and calibrate the instrument. When we started we would have liked to find such a condensed and structured compilation.

Table 1: Totals are not weighted by areas! Area 0-50 m is much smaller than that in 50-150 m, which is smaller than 150-300 m.

You are right. We should have specified this before: 'The total represents a distance weighted average with an exponential decay towards more distant areas (approximating the exponential distance-weighting from Zreda et al. (2008)).'

Figure 2: support volume may be a better term here Added 'volume'.

Use of cosmic ray neutron sensors for soil moisture
 2 monitoring in forests

#### 3

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7

## 8 Abstract

9 Measuring soil moisture with cosmic ray neutrons is a promising technique for intermediate 10 spatial scales. To convert neutron counts to average volumetric soil water content a simple 11 calibration function can be used (the  $N_0$ -calibration of Desilets et al., 2010). The calibration is 12 based on soil water content derived directly from soil samples taken within the footprint of the sensor. We installed a cosmic-ray neutron sensor (CRS) in a mixed forest in the lowlands of 13 north-eastern Germany and calibrated it 10 times throughout one calendar year. Each calibration 14 with the No-calibration function resulted in a different CRS soil moisture time series, with 15 deviations of up to  $0.1 \text{ m}^3 \text{ m}^{-3}$  (24 % of the total range) for individual values of soil water content. 16 Also, many of the calibration efforts resulted in time series that could not be matched with 17 independent in situ measurements of soil water content. We therefore suggest a modified 18 calibration function with a different shape that can vary from one location to another. A two-19 point calibration was found to effectively proved to be adequate to correctly define the shape of 20 21 the modified calibration function if the calibration points were taken during both dry and wet conditions spanning at least half of the total range of soil moisture. The best results were obtained 22 when the soil samples used for calibration were linearly weighted as a function of depth in the 23 24 soil profile and non-linearly weighted as a function of distance from the CRS, and when the depth-specific amount of soil organic matter and lattice water content was explicitly considered. 25 The annual cycle of tree foliation was found to be a negligible factor for calibration because the 26

Kommentar [A1]: Ref3: give max deviation in absolute values and also as % of the total range

Kommentar [A2]: Ref3: change to "correctly to define"

variable hydrogen mass in the leaves was small compared to the hydrogen mass changes by soil
moisture variations. As a final point, we provide a best-practice calibration guide for CRS in
forested environments.

30

# 31 1. Introduction

Determining average soil moisture content over larger areas is difficult, mainly for two reasons. 32 Firstly, soil moisture can be highly variable even at small spatial scales, especially under 33 34 intermediate wetness conditions (e.g. Western et al., 2004). Secondly, most common in situ measurement techniques only yield point measurements. To obtain a valid estimate of area-35 average soil moisture one needs to collect data from numerous locations within a given area. This 36 37 can be time-consuming and expensive. More recently, remote sensing of soil moisture at larger scales has become a research focus (e.g. see Ochsner et al., 2013 for a recent review); however, 38 the measurement depth of many of these methods is still limited to the upper 5 cm of the soil. 39 40 Also, both spatial and temporal resolution is rather coarse. A technique that intends to bridge the scale gap between point measurements of soil moisture and remote sensing is the use of cosmic 41 ray neutrons as indicators of soil moisture. A detailed description of the cosmic ray neutron 42 sensors (CRS) can be found in Zreda et al. (2008, 2012), here we will only describe the basic 43 measurement principle. Cosmic ray neutrons on Earth are formed when high-energy protons 44 deriving from galactic sources (such as supernovae) enter the Earth's atmosphere. Once in the 45 atmosphere, the protons interact with atomic nuclei (mainly nitrogen and oxygen) producing 46 cascades of secondary neutrons (also called high-energy neutrons) that travel towards the Earth's 47 surface and into the soils. When secondary neutrons interact with air or soil nuclei they trigger 48 the release (evaporation) of fast (but low energy) neutrons. The number of fast neutrons above 49 the soil surface depends strongly on the number of hydrogen atoms in the surroundings because 50 hydrogen atoms have a very high capacity to moderate fast cosmic ray neutrons (that means to 51 52 slow them down and turn them into thermal neutrons with even less energy - effectively removing the fast neutrons from the system). The number of hydrogen atoms increases with 53 increasing soil water content and hence soils with high water contents re-emit fewer fast neutrons 54 55 than soils with low water content. That leads to fewer fast neutrons being detected above-ground by the CRS which is generally installed 1-2 m above the soil surface. 56

Kommentar [A3]: Ref1: neutrons interact with air and soil nuclei

**Kommentar [A4]:** Ref3: "fast neutrons" means specific energy (around 1 MeV), so there is no need to qualify this.

As early as 1966 Hendrick and Edge reported that the intensity of fast (low-energy) neutrons 57 58 (~1 keV) detected above the ground depended on the hydrogen content of the soil, and Kodama (1985) found an inverse correlation of neutron intensity and soil moisture content with a neutron 59 60 sensor buried in the soil. In 2008, Zreda et al. introduced a method to measure average soil water content over a larger area (~30 ha) with CRS. The footprint of CRS, i.e. the area around the 61 sensor where 86 % of detected neutrons originate from, covers a circle with an approximate 62 radius of 300 m (Desilets and Zreda, 2013). However, the radius can decrease with increasing air 63 density and humidity, with increasing vegetation density and with increasing soil moisture to 64 65 about 100 m (Köhli et al., 2015). The effective measurement depth of CRS, i.e. the soil depth where 86 % of detected neutrons originate from, varies between 10 and 70 cm below surface 66 (Zreda et al., 2008), depending on soil type, water content and distance from the sensor (Köhli et 67 al., 2015). To account for the contributions of neutrons from different soil depths, various depth-68 69 weighting approaches have been proposed, some of them assuming a linear decrease of weights with depth (Franz et al., 2012a), others assuming a non-linear decrease with depth (Köhli et al., 70 2015). 71

The original measurement method uses a relationship between neutron flux and volumetric soil 72 water content with the shape of the relationship being known from neutron transport simulations. 73 For this relationship, Desilets et al. (2010) presented an equation with three constant shape 74 parameters  $(a_0, a_1, a_2)$  and one calibration parameter  $(N_0)$  which has to be calibrated with soil 75 moisture values determined by the gravimetric method from field soil samples. The influence of 76 soil lattice water and soil organic matter on the signal was investigated by Zreda et al. (2012). 77 They found that both lattice water and soil organic matter contain fixed amounts of hydrogen that 78 further attenuate the neutron signal and need to be taken into account. Lattice water and soil 79 organic matter corrections to the original relationship by Desilets et al. (2010) are provided for 80 81 example in Lv et al. (2014).

Other external factors influencing the neutron count that need to be corrected for are (a) atmospheric pressure (Bachelet et al., 1965), (b) incoming neutron flux (see e.g. Zreda et al., 2012, Bogena et al., 2013) and (c) specific humidity (Rosolem et al., 2013). More recently, the effects of biomass on the neutron signal have been discussed. Bogena et al. (2013) noted that aboveground biomass reduced the neutron count rate and thus decreased the sensitivity of the

sensor. To counter this loss of sensitivity they recommended a 24 h integration time for their 87 88 forested catchment as a compromise between decreased uncertainty and decreased time resolution. Hawdon et al. (2013) and Baatz et al. (2015) compared neutron counts for locations 89 with different amounts of biomass. Hawdon et al. (2013) reported that the variation in biomass 90 could explain 80 % of the variation in neutron counts when assuming a nonlinear relationship 91 between biomass and neutron counts, Baatz et al. (2015) explained 87 % of the variation 92 proposing a linear relationship between the two variables. Baroni and Oswald (2015) suggested 93 94 that the influence of above-ground biomass between the sensor and the ground which decreases 95 the effective measurement depth of the CRS can be incorporated into the weighting approach of 96 Franz et al. (2012a). This is especially important in locations where frequent large biomass changes occur, for example in agricultural fields. Coopersmith et al. (2014) found that soil 97 98 moisture in a corn crop is often overestimated when the leaf area index (LAI) is relatively high 99 while it is underestimated when LAI is relatively low - circumstances which could cause differences in the calibration and resulting soil moisture measurements. The influence of the litter 100 layer in forested environments was investigated by Bogena et al. (2013). Water content in the 101 litter layer changes rapidly and adds additional temporal variability to the CRS time series 102 complicating the extraction of the soil moisture signal. Therefore, Bogena et al. (2013) 103 recommended considering the water dynamics in the litter layer explicitly in the calibration 104 105 approach. Franz et al. (2013) introduced a new approach (the universal calibration function) that takes into account all sources of hydrogen thereby requiring estimates of lattice water, soil 106 organic carbon, and vegetation biomass as well as a regression factor that can be derived from 107 calibration or may directly be retrieved from neutron count measurements over a large water 108 body (500 m on all sides and deeper than 1 m). 109

Since the launch of the cosmic ray neutron method many changes and corrections have been 110 brought forward that altered the way the method is applied. These changes and corrections can be 111 divided into two groups. On the one hand, there are corrections that are applied to the raw 112 neutron count in order to remove the influence of other variables (such as air pressure and 113 114 humidity variations or fluctuations in incoming neutron counts). On the other hand, changes have been made to the way we average the soil moisture measurements during the calibration 115 campaigns in order to get a representative soil moisture value that corresponds to what the sensor 116 actually "sees" at the time of calibration (changing effective measurement depth, changing 117

footprint diameter, inclusion of lattice water and soil organic matter water equivalent). All this 118 119 has led to improvements in the method's accuracy for many environments. Most of these studies were performed in medium to high-count environments with neutron count rates above 1000 120 counts per hour, in generally dry environments, at higher elevations and with little vegetation. 121 122 Only a few studies were performed in low-count environments with count rates below 1000 counts per hour (e.g. Rivera Villareyes et al., 2011; Bogena et al., 2013). In the present study, we 123 evaluated whether the CRS also provides reliable and consistent soil moisture measurements in a 124 low-count environment, i.e., in a temperate mixed forest close to sea level. We tested several 125 126 weighting approaches to convert gravimetrically determined soil water content of the top 30 cm 127 into an average soil water content that can be used for the calibration of the CRS. Additionally, we analyzed whether the annual forest cycle of foliation and defoliation is important to consider 128 129 for instrument calibration. We furthermore compiled a best-practice for the calibration of CRS in 130 forested, low-count environments which is provided in Appendix A.

131

# 132 2. Field site and instrumentation

The CRS (CRS-1000 by Hydroinnova) was installed in late 2013 in the Müritz National Park in 133 north-eastern Germany (53°19'49.0"N, 13°11'56.5"E) at an elevation of about 84 m a.m.s.l. (Fig. 134 1, inset). Precipitation, temperature and relative humidity data was provided by the climate 135 station Serrahn (1.6 km to the north). Average annual air temperature at the site is 8°C with a 136 maximum in July (17.2°C) and a minimum in January (-0.9°C). Average annual precipitation is 137 580 mm with a maximum in June (65 mm) and a minimum in February (28 mm). This makes for 138 a maritime temperate climate (Cfb) in the Köppen climate classification. The sensor is located in 139 140 a sandy outwash plain, a relic from the last glaciation, which causes the soil texture to be homogeneous with sand fractions of about 95% throughout the entire profile. Data from a nearby 141 well shows that the groundwater level at the site is almost 20 m below the terrain surface. The 142 vegetation within the sensor footprint consists of both deciduous and coniferous trees. 143 Immediately surrounding the sensor is a mature beech forest (Fagus sylvatica L., older than 100 144 years), also within the footprint (but farther away) with a distance of at least 40 m from the sensor 145 there is young pine (Pinus sylvestris L.), oak (Quercus robur L.) and spruce (Picea abies (L.) 146 H.Karst.) forest (all younger than 50 years) as well as a small strip of open grassland (see Fig. 1 147 5

and also Fig. 3 for a map of the forest stands and Table 1 for fractions of the different tree stands
within the footprint). Depending on the tree species, the mineral soil is covered by an organic soil
layer and a litter layer of variable depth and water holding capacity.

For validation of the CRS soil water content measurements, in May of 2014 we installed 18 soil 151 152 moisture sensors (TOMST) close to the soil sampling/calibration locations. They are based on the principle of time domain transmission (TDT) and each sensor comes with its own logger and 153 power supply (more information under: http://www.tomst.cz/tms/TMS-3.html). These sensors 154 155 were installed vertically from the terrain surface into the soil so that they continuously measure soil water content averaged over the top 16 cm of the soil. In order to calibrate the sensors we 156 used the gravimetric soil moisture data we collected from the upper 15 cm during the last five 157 calibration campaigns which were carried out within the measurement period of the sensors 158 159 (June-November 2014). The volumetric water content within the upper 15 cm of the CRS 160 footprint was calculated as the mean of all 18 TDT sensors.

161

#### 162 3. Methods

#### 163 **3.1. Calibration**

164 We conducted a total of 10 calibration campaigns throughout one calendar year (2014). The first one (WI) took place in February during winterly conditions with very wet soils. The next four 165 calibrations (S1-4) followed in spring (April-May) and covered the entire period of tree foliation. 166 The sixth calibration (SU) was done under very dry conditions in July and the last four 167 calibrations (F1-4) in fall (October-November) covering the trees' defoliation. For all the 168 calibration campaigns we followed the recommended sampling pattern for the calibration of CRS 169 which was developed by Zreda et al. (2012) and slightly modified and detailed in Franz et al. 170 (2012b). The sampling pattern prescribes 3 concentric circles around the CRS with radii of 25, 75 171 172 and 200 m, respectively (Fig. 1). The 3 circles are intersected by 6 straight lines that point from 173 the sensor towards north  $(0^\circ)$ , north-east  $(60^\circ)$ , south-east  $(120^\circ)$ , south  $(180^\circ)$ , south-west  $(240^\circ)$ and north-west (300°). Samples are taken in the vicinity of all intersections – the samples do not 174 have to be taken at the exact spot of the intersection. This sampling pattern ensures that each 175

sample has equal weight towards the spatial mean of soil moisture that is detected by the CRS, 176 177 assuming that the sensitivity of the CRS decreases exponentially with distance. We used a splittube sampler to extract 30 cm soil cores at 18 locations within the footprint of the sensor 178 179 afterwards dividing each soil core into six 5 cm thick soil samples. For each of the 10 calibrations this left us with 108 soil samples which were then transferred in sealed plastic bags to the 180 laboratory where they were immediately weighed, then oven-dried at 105°C for 24 h and then 181 weighed again to determine their volumetric water content and bulk density. Afterwards, lattice 182 183 water, soil organic matter content and root biomass were determined for six depth-representative 184 soil samples. To this end the 108 samples (taken from the last calibration campaign in November) 185 were grouped by sampling depth. We extracted 2 g from each of the 18 samples per sampling depth and combined them to create one bulk sample per depth. Then, the already oven-dried 186 samples were weighed and put in the oven for another 24 h at a temperature of 400°C. The 187 188 procedure is called 'loss on ignition' since the organic matter is burned off during the process (Ball, 1964; Davies, 1974). This removed most of the soil organic matter and root biomass from 189 the samples. After weighing the samples (to compute the fraction of combined soil organic matter 190 and root biomass) they were again placed in the oven for 24 h, this time at a temperature of about 191 1000°C. After that, the lattice water was also removed from the samples. A final weighing 192 yielded the fraction of lattice water per soil depth. In order to make soil organic matter and root 193 194 biomass comparable to the influence of pure water we converted them into equivalents of water by multiplying their weight by 0.556 which is the ratio of five times the molecular weight of 195 water to the molecular weight of cellulose (taking into account that cellulose ( $C_6H_{10}O_5$ ) contains 196 10 hydrogen atoms per molecule while water (H<sub>2</sub>O) only contains two) (Hawdon et al., 2014). 197

The neutron counts from the sensor were smoothed with a 12 h moving window to reduce measurement noise (see Bogena et al., 2013). The next step was to correct the neutron counts for variations in (a) pressure, (b) incoming neutron flux and (c) water vapor in the air. This was done by applying the following corrections:

202 a. Pressure correction:

203 
$$N_p = N_{raw} * e^{\left(\frac{x-x_0}{L}\right)}$$
(1),

with  $N_p$  being the pressure corrected neutron counts (counts h<sup>-1</sup>),  $N_{raw}$  the raw neutron counts 204 (counts  $h^{-1}$ ), x the atmospheric shielding depth (g cm<sup>-2</sup>) for every time step (derived from 205 atmospheric pressure measured directly inside the CRS case),  $x_0$  the average atmospheric 206 shielding depth (g cm<sup>-2</sup>) for the entire measurement period and L the effective nucleon 207 attenuation length for high-energy neutrons (for our site we assumed a value of 135.9 g cm<sup>-2</sup> 208 which is equivalent to 133.3 hPa) (Desilets and Zreda, 2003). To convert atmospheric pressure 209 (hPa) into shielding depth (g cm<sup>-2</sup>) the atmospheric pressure has to be multiplied by 1.0194 s<sup>2</sup> m<sup>-2</sup> 210 1 211

b. Incoming flux correction (Zreda et al., 2012):

213 
$$N_{pi} = N_p * \frac{N_{avg}}{N_{nm}}$$
(2),

with  $N_{pi}$  being the sensor neutron count rate corrected for changes in atmospheric pressure and incoming neutrons (counts h<sup>-1</sup>),  $N_{avg}$  the average count rate of incoming neutrons (counts h<sup>-1</sup>) over the entire measurement period and  $N_{nm}$  the neutron count rate of the neutron monitor for each time step (counts h<sup>-1</sup>).

As the time series of the closest neutron monitor, located in Kiel, Germany, contains several data gaps, we selected the continuous time series of the Jungfraujoch, Switzerland, for this study. We scaled this time series by adjusting its mean (309 counts  $h^{-1}$ ) to the mean of the Kiel time series (327 counts  $h^{-1}$ ). The resulting time series resembles the Kiel time series very closely (Fig. S1).

222 c. Water vapor correction (Rosolem et al., 2013):

223 
$$N_{pih} = N_{pi} * \left[ 1 + 0.0054 * \left( p_{v0} - p_{v0}^{ref} \right) \right]$$
 (3),

with  $N_{\text{pih}}$  being the sensor neutron count corrected for changes in pressure, incoming neutrons and water vapor (counts h<sup>-1</sup>),  $p_{v0}^{\text{ref}}$  the average absolute humidity of the air over the entire measurement period (g m<sup>-3</sup>) and  $p_{v0}$  the absolute humidity for each time step (g m<sup>-3</sup>). The constant 0.0054 has units of m<sup>3</sup> g<sup>-1</sup>.

Finally, to convert corrected neutron counts  $(N_{\text{pih}})$  into volumetric soil moisture ( $\theta$ ), Desilets et al. (2010) introduced an equation with four parameters – three of which ( $a_0 = 0.0808$ ,  $a_1 = 0.372$ ,  $a_2$  = 0.115) were determined via neutron transport simulations and a fourth one (N<sub>0</sub>) that serves as a calibration parameter accounting for site and sensor specific variations and representing neutron counts over dry soil at reference conditions during calibration. <u>Calibration has to be performed</u> using the total belowground hydrogen pool (including hydrogen contributions from lattice water (W<sub>L</sub>), soil organic matter (SOM) and root biomass (B<sub>R</sub>)). Soil water content is then computed by subtracting the other hydrogen pools from the measured neutron-derived signal:

236 
$$\theta(t) = \left\{ \left[ a_0 * \left( \frac{N_{pih}(t)}{N_0} - a_1 \right)^{-1} - a_2 \right] * \rho_{bd} \right\} - W_L - (SOM + B_R)$$
(4).

The other parameters  $\rho_{bd}$ ,  $W_L$ , SOM and  $B_R$  can be measured directly from the calibration soil 237 samples: the bulk density of the soil ( $\rho_{bd}$  in g cm<sup>-3</sup>), the summed volume fraction of lattice water 238 in the soil grains and tightly bound water ( $W_L$  in m<sup>3</sup> m<sup>-3</sup>), the combined volume fraction of soil 239 organic matter and root biomass water equivalent ( $SOM+B_R$  in m<sup>3</sup> m<sup>-3</sup>). In order to calibrate the 240 sensor one first has to determine the depth- (and distance-) weighted averages for  $ho_{\rm bd}, W_{\rm L},$ 241  $SOM+B_R$  and  $\theta$  as well as  $N_{pih}$  (averaged over 12 h) for the time of calibration. This is necessary 242 because several factors can influence the effective measurement depth  $z^*$  (which is the depth of 243 the soil layer up to which 86 % of the neutrons that the CRS detects originate from) and the 244 footprint size of the sensor (Fig. 2). Afterwards  $N_0$  is adjusted iteratively (e.g. with a simple 245 246 Solver routine in Microsoft Excel) until the right-hand side of the equation equals the left-hand 247 side.

We tested four soil moisture weighting approaches (Table 2), described in detail below, to determine which information is necessary for an accurate calibration.

1. In the first approach (simple depth-weighting, SDW) a linear depth-weighting function was used (Franz et al., 2012b), where wt(z) represents the weight that is applied to the soil moisture measurements from a certain soil depth *z*:

253 
$$\begin{cases} wt(z) = a \left[ 1 - \left( \frac{z}{z^*} \right)^b \right] & 0 \le z \le z^* \\ wt(z) = 0 & z > z^* \end{cases}$$
(5),

254 where

255 
$$a = \frac{1}{z^* - \frac{z^{*b+1}}{(b+1)z^{*b}}}$$

256 and

257 
$$z^* = \frac{5.8}{H_p + 0.0829}$$
 (7)

258 and

 $259 \qquad H_p = W_L + SOM + B_R + \theta$ 

In these equations z is the soil depth below the surface in cm and  $z^*$  is the effective measurement 260 261 depth in cm, a is a parameter that ensures that the weights are conserved, b controls the curvature of the weighting function and equals 1 for linear weighting,  $H_p$  is the water equivalent of the 262 belowground hydrogen pools (m<sup>3</sup> m<sup>-3</sup>),  $W_L$  is lattice water (m<sup>3</sup> m<sup>-3</sup>), SOM is soil organic matter 263 water equivalent (m<sup>3</sup> m<sup>-3</sup>),  $B_R$  is root biomass water equivalent (m<sup>3</sup> m<sup>-3</sup>) and  $\theta$  is the 264 gravimetrically determined volumetric soil pore water content (m<sup>3</sup> m<sup>-3</sup>). The original approach by 265 Franz et al. (2012b) was modified by Bogena et al. (2013) using the total hydrogen content of 266 267 belowground hydrogen pools  $H_p$  instead of just using the volumetric soil water content  $\theta$ . Since  $H_{\rm p}$  changes with soil depth we used an iterative approach to determine the appropriate weights. 268 Starting with an average value for the upper 30 cm of the soil we computed an effective 269 270 measurement depth  $z^*$  and weighted  $H_p$  of the different soil depths accordingly. With this new value of  $H_p$  we then recomputed  $z^*$  and the weights. Usually the value of  $H_p$  stabilizes after a few 271 iterations. The bulk density ( $\rho_{bd}$ ) of the soil changes with depth and influences the soil moisture 272 measurements too. Therefore it was also being taken into account during the iterative process of 273 determining the effective measurement depth  $z^*$  and the weighted soil moisture. In this first 274 weighting approach we did not use our depth-specific measurements of  $W_L$  and  $SOM+B_R$ , instead 275 we assumed an average weight fraction value of combined  $W_L+SOM+B_R$  for the entire 30 cm 276 profile. 277

278 2. The second approach (depth-specific weighting, DSW) was identical to the first one (SDW)

except for using depth-specific measurements of  $W_L$  and  $SOM+B_R$  (see Table 3 for an example).

(6),

(8).

3. For the third approach (distance-depth-weighting, DDW), we adopted the weighting approach described in Köhli et al. (2015). This approach introduces distance-dependent variable depthweighting where the effective measurement depth decreases with distance from the sensor. The effective measurement depth  $z^*$  is calculated according to:

284 
$$z^* = \rho_{bd}^{-1} \left[ 8.32 + 0.14 * \left( 0.97 + e^{\frac{-r}{100}} \right) * \frac{26.42 + H_p}{0.057 + H_p} \right]$$
 (9),

where  $\rho_{bd}$  is the bulk density of the soil (g cm<sup>-3</sup>), *r* is the radial distance (in meters) from the CRS and  $H_p$  is the water equivalent of the belowground hydrogen pools (m<sup>3</sup> m<sup>-3</sup>) (see Eq. 8). This approach also assumes that the footprint size of the sensor varies with soil water content and atmospheric water content. We computed the varying footprint diameter for each calibration campaign and weighted the samples from 25, 75 and 200 m accordingly.

4. The fourth approach (distance-depth-weighting, non-linear, DDWnl) was identical to the third
one (DDW) except for using the non-linear depth-weighting function recommend by Köhli et al.
(2015) instead of the linear one (from Eq. 5):

293 
$$wt(z) = e^{\frac{-2z}{z^*}}$$
 (10).

# 294 3.2. Estimation of biomass and influence of seasonal changes in biomass

Biomass influences neutron counts due to its hydrogen content. In order to test (and potentially
exclude) the influence of seasonal changes in aboveground forest biomass, we estimated living
tree biomass and tree biomass changes throughout the year by applying the aboveground dry
biomass functions for beech forest (*Fagus sylvatica* L.) from Santa Regina et al. (1997):

299 
$$B_S = 0.0894 * DBH^{2.4679}$$
 (11),

$$300 \quad B_B = 0.0317 * DBH^{2.3931} \tag{12},$$

$$301 \quad B_L = 0.0145 * DBH^{1.9531} \tag{13}.$$

B<sub>S</sub> is dry stem biomass (kg tree<sup>-1</sup>),  $B_B$  dry branch biomass (kg tree<sup>-1</sup>),  $B_L$  dry leaf biomass (kg tree<sup>-1</sup>) and *DBH* is the diameter of the tree stem at breast height (cm). Total dry above-ground biomass  $B_{ag}$  is the sum of the three components.

To apply these functions we conducted a survey of tree diameters and tree density in the beech 305 306 forest that surrounds the CRS. This allowed us to determine both the total biomass of the beech forest, as well as the seasonally variable fraction of biomass (leaf biomass divided by total 307 biomass). We first calculated the water mass  $(W_{agb})$  in stems, branches and leaves (assuming a 308 309 leaf water content of 0.6 kg per kg of wet biomass (Gravano et al., 1999) and a wood water content of 0.11 kg kg<sup>-1</sup> (Bouriaud et al., 2004)). Finally, using the mass fraction of hydrogen in 310 water ( $M_w = 0.1119$  kg H per kg H<sub>2</sub>O) and in dry biomass ( $M_b = 0.0622$  kg H per kg Cellulose: 311 312  $C_6H_{10}O_5$ ) the total hydrogen mass ( $H_{agb}$ ) of above-ground biomass in the beech stand was 313 derived:

314 
$$H_{aab} = W_{aab} * M_w + B_{aa} * M_b$$
 (14).

We did not conduct surveys on the other tree species. Table 1 shows that the beech stand covers 56% of the footprint area around the CRS (when assuming the exponential distance-weighting from Zreda et al. (2008)). Pine covers 16%, spruce 13%, oak 8%. With the new distance weighting function of Köhli et al. (2015), the cover fractions of the other tree species would decrease even further. Also, the seasonal variation in spruce and pine above-ground biomass is very small and thus we consider it to be constant in this study.

## 321 3.3. Validation

As an objective performance measure to compare the soil moisture time series derived from the CRS with the soil moisture time series from the TDT sensors we used the modified Kling-Gupta efficiency KGE' (Gupta et al., 2009; Kling et al., 2012):

325 
$$KGE' = 1 - \sqrt{(r-1)^2 + (\beta - 1)^2 + (\gamma - 1)^2}$$
 (15).

326 With correlation coefficient *r*:

327 
$$r = \frac{\sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n} (x_i - \bar{x})^2 * \sqrt{\sum_{i=1}^{n} (y_i - \bar{y})^2}}}$$
(16),

bias ratio  $\beta = \mu_{mod}/\mu_{obs}$  and variability ratio  $\gamma = (\sigma_{mod}/\mu_{mod})/(\sigma_{obs}/\mu_{obs})$ . The KGE' measures the Euclidian distance in a 3-D space where the correlation coefficient *r* is on one axis, the variability ratio  $\beta$  is on the second axis and the bias ratio  $\gamma$  is on the third axis. KGE' scores range from 1 (representing a perfect fit) to  $-\infty$ . Due to the composite nature of the KGE' it is relatively simple to analyze which feature of the time series (correlation, bias, variability) contributes most to the good/bad performance of a model.

334

### 335 **4. Results**

# 336 4.1. Gravimetric soil water measurements and soil physical characteristics

Soil water content in the sandy soils ranged between 0.03 and 0.37 m<sup>3</sup> m<sup>-3</sup> (absolute minimum 337 and maximum values of individual soil core samples during the 10 sampling campaigns). The 338 spatial distribution of volumetric soil water content for the 10 calibration days is shown in Fig. 3. 339 At each location the soil water content is an unweighted average value of the six samples taken 340 from 0 to 30 cm depth. The mean volumetric soil water content for the calibration days over all 341 calibration locations ranged from 0.07 up to 0.16 m<sup>3</sup> m<sup>-3</sup> with standard deviations ranging from 342 0.015 to 0.047 m<sup>3</sup> m<sup>-3</sup>. The depth and distance weighted averages used for calibration ranged 343 from 0.08 to 0.24 m<sup>3</sup> m<sup>-3</sup> (see for example Table 4, column:  $\theta_{depthW}$ ). A general soil moisture 344 pattern emerged with the soil moisture under coniferous tree stands being lower and under 345 deciduous tree stands being higher. Especially the uppermost soil layer (0-5 cm) was drier under 346 the coniferous trees - on average about 0.065 m<sup>3</sup> m<sup>-3</sup> - while the deeper soil layers under 347 coniferous trees were about 0.023 m<sup>3</sup> m<sup>-3</sup> drier. The highest spatial variabilities in soil moisture 348 were encountered during spring and fall seasons and more homogenous soil moisture conditions 349 350 during winter and summer. The wettest calibration we conducted (WI) yielded an average soil water content of 0.29 m<sup>3</sup> m<sup>-3</sup> for the top 5 cm. Calibration at higher soil water content is difficult 351 as it only occurs for short periods of time after large precipitation events when significant 352 353 amounts of intercepted water are also present in the canopy and litter layer.

The average bulk density ( $\rho_{bd}$ ) measurements for the 10 calibration campaigns ranged from 1.16 to 1.22 g cm<sup>-3</sup> (mean: 1.18 g cm<sup>-3</sup>, standard deviation: 0.02 g cm<sup>-3</sup>). The weight fraction of soil organic matter and root biomass water equivalent (w*SOM*+*B*<sub>R</sub>) was determined to be 51.4 g kg<sup>-1</sup> in the shallowest soil layer (0-5 cm) with decreasing values at depth. The weight fraction of lattice water (w*W*<sub>L</sub>) was determined to be 3.2 g kg<sup>-1</sup> in the shallowest soil layer with slightly increasing values at deeper soil depths.

#### 360 **4.2. Footprint variability**

The footprint diameters calculated according to Köhli et al. (2015) and used in approaches 3 and 361 362 4 ranged from 185 m for the wettest to 200 m for the driest conditions. This resulted in distance weights of ~0.56 (for samples from 25 m distance), ~0.35 (for samples from 75 m distance) and 363 364  $\sim 0.10$  (for samples from 200 m distance). These weighting factors varied only marginally between the individual calibration campaigns despite considerable differences in soil and 365 atmospheric water content. Sampling distances with equal weights according to Köhli et al. 366 (2015) would have differed from our sampling pattern (~1 m, ~33 m, ~140 m instead of 25 m, 75 367 m, 200 m), a condition which we balance by adjusting the distance weights. Furthermore the 368 conditions within 30 m around our CRS are quite homogenous since the sensor is located within 369 370 a pure beech stand and we are expecting little difference in average soil moisture content between locations at 1 and 25 m distance. 371

#### 372 4.3. Calibration

373 The average reference atmospheric pressure  $(P_0)$  for the entire measurement period was 1005.8 hPa; the average reference incoming neutron flux ( $N_{avg}$ ) was 328.3 counts h<sup>-1</sup>; the average 374 reference absolute humidity  $(p_{v0}^{ref})$  was 9.1 g m<sup>-3</sup>. Equations (5) through (10) were used to 375 calculate depth-weighted volumetric soil water content  $\theta_{depthW}$  and depth-weighted water 376 equivalent of belowground hydrogen pools (Hp)depthW according to the four weighting approaches 377 we applied. Equations (1)-(3) were used to compute  $N_p$ ,  $N_{pi}$  and  $N_{pih}$ , and then Eq. (4) to identify 378  $N_0$  for each calibration. Table 3 provides an example of the depth-weighting following approach 379 2 (DSW with depth-specific values of  $W_{\rm L}$  and  $SOM+B_{\rm R}$ ). 380

The values in Table 3 result in a depth-weighted average volumetric water content  $\theta_{depthW}$  of 0.150 m<sup>3</sup> m<sup>-3</sup>, a depth-weighted water equivalent of belowground hydrogen pools ( $H_p$ )<sub>depthW</sub> of 0.179 m<sup>3</sup> m<sup>-3</sup> and a depth-weighted bulk density ( $\rho_{bd}$ )<sub>depthW</sub> of 0.981 g cm<sup>-3</sup>. If  $W_L$  and  $SOM+B_R$ were not considered, the values for  $\theta_{depthW}$  and ( $\rho_{bd}$ )<sub>depthW</sub> would change to 0.146 m<sup>3</sup> m<sup>-3</sup> and 1.013 g cm<sup>-3</sup> respectively, because the effective measurement depth  $z^*$  increases when the higher amounts of  $SOM+B_R$  in the shallow layers are not considered, thus giving more weight to low soil moisture values in deeper soil horizons.

Table 4 lists the parameters relevant for calibration for all 10 calibration dates (again following approach 2, DSW, with depth-specific values of  $W_L$  and  $SOM+B_R$ ).

Following the standard  $N_0$ -calibration approach of Desilets et al. (2010), we should have ended up with the same  $N_0$  value for each of the 10 calibrations. However, the  $N_0$  range we found was considerable – e.g. from 808 to 895 counts h<sup>-1</sup> for the DDW approach (mean: 841.9 counts h<sup>-1</sup>, standard deviation: 13.7 counts h<sup>-1</sup>). As a consequence, the 10 computed time series also showed differences in volumetric soil water content (Fig. 4 illustrates results for the DDW approach). In the most extreme case, these differences were larger than 0.1 m<sup>3</sup> m<sup>-3</sup> (which is equal to 24 % of the total range of soil water content at the site).

In fact, none of the four weighting approaches was able to solve the problem of determining a unique calibration parameter for our field site. All weighting approaches resulted in largely deviating  $N_0$ -values between the individual calibrations (see means and standard deviations in column 1 and 2 of Table 5). This in turn led to differences in the resulting time series of volumetric soil water content (see means and standard deviations in column 3 and 4 of Table 5).

## 402 4.4. Modified calibration function

To include all information of our 10 calibration campaigns into our analysis, we fitted modified calibration functions to four sets of 10 calibration points derived from the four different weighting approaches (see section 3.1). This was done by using the Microsoft Excel Solver software to optimize the three shape parameters ( $a_0$ ,  $a_1$ ,  $a_2$ ) and  $N_0$  through the calibration point cloud (solid lines in Fig. 5). Plotting the  $N_{pih}$ -values of all 10 calibrations against the gravimetrically determined and depth- (and distance-) weighted volumetric soil moisture revealed

that the standard shape of the soil moisture-neutron count relation is not valid at our field site. 409 410 Instead of plotting along functions defined by the standard calibration (Desilets et al., 2010) (examples are dotted lines in Fig. 5) our calibration points are better captured by less steep 411 functions (solid lines in Fig. 5 are the best-fit calibration functions for the different approaches). 412 Using the  $N_0$ -calibration function with the standard shape parameters may lead to large soil water 413 content deviations between individual calibration campaigns, especially under wet soil moisture 414 conditions. The slope of the  $N_0$ -calibration function is essentially too steep, which means that in 415 our environment a change in the neutron count is caused by a more subtle change in soil moisture 416 417 than is assumed by the standard relationship - essentially the sensor has a higher resolution/sensitivity than one would expect. 418

The optimized parameters for the four approaches are shown in Table 6. The resulting soilmoisture time series are shown in Fig. 6.

#### 421 **4.5. Validation**

422 We tested whether the modified calibration functions improved the performance of the CRS measurements relative to in situ measurements, and if so, which of the weighting approaches 423 performed best. In order to do that we compared the soil moisture time series from the CRS 424 (using the standard  $N_0$ -calibration function from Desilets et al. (2010) and applying our newly 425 derived corrected relationships) with the soil moisture time series from the TDT sensors 426 distributed throughout the footprint. As a first step, the CRS measurements had to be converted to 427 428 a soil water content value representative of the top 15 cm of the soil (the integration depth of the TDT sensors). For this purpose we compared the weighted volumetric water content ( $\theta_{depthw}$ ) 429 from the gravimetric measurements of the calibration campaigns (basically what the CRS is 430 431 supposed to "see") with the unweighted average gravimetric measurements of the top 15 cm  $(\theta_{15cm})$  (Fig. S2). We found strong linear correlations for two of the weighting approaches (SDW 432 and DSW) with CRS water content being larger than the  $\theta_{15cm}$  values and increasing differences 433 for wetter soil conditions (indicating that for higher soil moisture the CRS overestimates soil 434 435 water contents in the top 15 cm while for lower soil moisture the overestimation decreases). For approaches 3 and 4 (DDW and DDWnl) offsets of 0.006 and 0.011 m<sup>3</sup> m<sup>-3</sup> indicated slightly 436 437 lower weighted soil water content than the unweighted top 15 cm values. The linear correlations Kommentar [A5]: Ref1: delete "resolution"

for the first two weighting approaches were expected since when it is wetter, the effective 438 439 measurement depth is reduced for the CRS measurements and the wetter shallower soil layers receive more weight. Therefore, the CRS measurements result in higher soil water content than 440 the gravimetric measurements. However, it seems that in approaches 3 and 4 the distance 441 weighting counters this effect. A probable explanation is that the formula used for the distance-442 depth weighting increases the effective measurement depth. This causes higher weights for 443 deeper (drier) soil layers even under wet conditions and could counteract the trend. We then 444 converted the CRS time series by the above relationships into time series that were representative 445 446 of the top 15 cm and compared them to the TDT measurements. The modified Kling-Gupta 447 efficiency (KGE') was used as a performance measure. The worst performance was achieved by the simple depth weighting approach (KGE'(SDW) = 0.83, Table 7), the performance improved 448 when depth-specific weighting was included (KGE'(DSW) = 0.88) and it further improved when 449 450 including distance weighting (KGE'(DDW) = 0.89). The linear depth weighting worked better than the non-linear depth weighting (KGE'(DDWnl) = 0.83). That means that the distance-depth-451 weighting approach (DDW) improved the neutron sensors performance the most. In comparison, 452 using the single-point standard N<sub>0</sub>-calibration function and DDW yielded KGE's for the 453 individual calibration campaigns ranging from 0.58 to 0.83 with a mean KGE' of 0.71 ( $\pm$ 0.08). It 454 is important to note that all of the modified calibration approaches performed better than their 455 standard calibration counterparts. The improvement of performance of the new N<sub>0</sub>-calibration 456 functions compared to the standard calibration functions was caused by the better agreement of 457 both the bias ratios  $\beta$  and the variability ratios  $\gamma$ , i.e. both the means and the variabilities of the 458 CRS time series better matched the TDT observations (see also Fig. 7). This supports the 459 hypothesis that at our field site larger than expected changes in neutron count are already caused 460 461 by subtle changes in soil moisture.

# 462 **4.6. Optimizing calibration efforts**

We further tested whether two or more individual calibration campaigns are required to determine a comprehensive calibration function shape, and under which soil moisture conditions these calibrations should be conducted. We paired each individual calibration point (derived from the best-performing weighting approach, DDW) with all the other calibration points (WI and S1, WI and S2, WI and S3, etc.) and computed best-fit calibration functions for all of these pairings(Fig. 8).

Then we used the resulting calibration functions to convert the measured neutron counts into time 469 series of volumetric soil water content and compared these to the TDT measurements (again 470 471 using the KGE' as the performance measure). We found that a two-point calibration proved to be sufficient in case that the difference in soil water content between the two calibrations was larger 472 than 0.1  $\text{m}^3 \text{m}^{-3}$  (i.e. for our sandy soils it covered ~50 % of the observed range of average soil 473 474 water content). Figure 9 indicates that the calibrated neutron count-soil water content conversion 475 will always perform well if the soil moisture difference between the two calibrations is sufficiently large. Also, it turned out to be more important to capture a calibration point at very 476 dry rather than at very wet soil water contents. This is illustrated in Fig. 9 where predominantly 477 478 calibrations that involve low soil water contents (red dots) as the minimum value achieve KGE's of 0.9 while these KGE' values are also achieved more frequently with intermediate soil water 479 contents (light blue dots) as the maximum value. 480

#### 481 **4.7. Variability of hydrogen pools**

The tree survey revealed a median diameter of 23.9 cm (Min: 3.2 cm, Q<sub>25</sub>: 11.5 cm, Q<sub>75</sub>: 43.7 cm, 482 Max: 93.3 cm) and a tree density of 0.05 stems m<sup>-2</sup>. With these values at hand and Eqs. (11)-(13) 483 the dry above-ground biomass of the beech stand  $(B_{ag})$  was 63.8 kg m<sup>-2</sup> (with 62.8 kg m<sup>-2</sup> from 484 stem and branches and 1.0 kg m<sup>-2</sup> from leaves) (Fig. 10). These values result in 9.2 kg m<sup>-2</sup> of 485 biomass water ( $W_{agb}$ ) (with 7.8 kg m<sup>-2</sup> from stem and branches and 1.5 kg m<sup>-2</sup> from leaves). 486 Further calculations yield a hydrogen mass of 4.8 kg m<sup>-2</sup> for stem and branches and a hydrogen 487 mass of 0.22 kg m<sup>-2</sup> for leaves (Eq.14). Other hydrogen pools within the CRS footprint were also 488 assessed. The thickness of the litter layer was determined to be 5 cm on average. Assuming a 489 porosity of 85 % yields a hydrogen mass of 0.47 kg m<sup>-2</sup> for a dry litter layer. Hence, the hydrogen 490 mass of the static biomass (stem, branches and dry litter) amounted to 5.24 kg m<sup>-2</sup>. Beech litter 491 was found to have a maximum interception capacity of 2.8 mm in a forest in Luxembourg 492 (Gerrits et al., 2010) corresponding to an additional 0.31 kg m<sup>-2</sup> of hydrogen when the litter layer 493 is wet. The canopy interception of beech can be assumed to be up to 1.5 mm (Gerrits et al., 2010) 494 (i.e. another 0.17 kg  $m^{-2}$  of hydrogen is added to the system when the canopy is wet). The 495

hydrogen contribution of soil organic matter and root biomass changes with soil water content 496 497 because the effective measurement depth of the sensor changes. Applying the DDW approach we computed a value of 0.36 kg m<sup>-2</sup> for wet conditions (0.29 m<sup>3</sup> m<sup>-3</sup>), a value of 0.44 kg m<sup>-2</sup> for 498 intermediate conditions (0.17 m<sup>3</sup> m<sup>-3</sup>) and a value of 0.66 kg m<sup>-2</sup> for dry conditions (0.05 m<sup>3</sup> m<sup>-3</sup>). 499 The hydrogen contribution of lattice water also changes with moisture conditions (wet: 0.05 kg 500 m<sup>-2</sup>; intermediate: 0.07 kg m<sup>-2</sup>; dry: 0.15 kg m<sup>-2</sup>). A pore water content of 0.29 m<sup>3</sup> m<sup>-3</sup> equals a 501 hydrogen mass of 4.12 kg m<sup>-2</sup>, a pore water content of 0.17 m<sup>3</sup> m<sup>-3</sup> equals a hydrogen mass of 502 3.26 kg m<sup>-2</sup> and a pore water content of 0.05 m<sup>3</sup> m<sup>-3</sup> reduces the hydrogen mass to 1.77 kg m<sup>-2</sup>. 503 504 Figure 11 and Table 8 give an overview of the different hydrogen pools for varying moisture 505 conditions within the footprint of the CRS.

506

#### 507 5. Discussion

# 508 5.1. Potential influences on neutron counts

The 10  $N_0$ -calibration parameters derived from our 10 calibrations varied considerably. In a first 509 analysis we found that this was not related to the different soil moisture conditions during 510 calibration. In search of other potentially unaccounted factors that influence the neutron count we 511 compared  $N_0$ -values obtained from the 10 calibrations with apparent atmospheric pressure, 512 specific humidity, temperature and estimates of forest crown cover (derived from photographs 513 taken from the ground aiming at the zenith) during the calibration campaigns. No seasonal or 514 other temporal relationships were found. The contributions of different hydrogen pools (Fig 11) 515 516 reveal that a large percentage of hydrogen at our field site stems from the above-ground vegetation (52 to 68 %, depending on moisture conditions). Fortunately, most of this hydrogen is 517 static in nature and can be accounted for by the calibration of the CRS. Assuming that the 518 hydrogen content of the stem and branches is constant and only the leaves change seasonally one 519 is left with a fraction of variable hydrogen in the above-ground biomass that accounts for 2-3 % 520 of the total hydrogen mass. The variability in hydrogen due to foliation and defoliation in the 521 beech forest surrounding the CRS amounts to 0.22 kg m<sup>-2</sup>. This means that it equals a change in 522 soil water content of about 0.031 m<sup>3</sup> m<sup>-3</sup> (under wet conditions) and 0.018 m<sup>3</sup> m<sup>-3</sup> (under dry 523 conditions). These differences for wet and dry conditions are due to the fact that the effective 524 19

measurement depth  $z^*$  of the CRS increases for dry conditions: the sensor receives the neutron 525 526 signal from deeper soil depths and therefore an equal increase in soil water content requires a larger amount of water since a larger soil column has to be filled. At high soil moisture, a 0.01 m<sup>3</sup> 527 m<sup>-3</sup> soil moisture change from 0.28 to 0.29 m<sup>3</sup> m<sup>-3</sup> equals a change of 0.07 kg m<sup>-2</sup> of hydrogen in 528 the soil. At low soil moisture the change from 0.05 to 0.06 m<sup>3</sup> m<sup>-3</sup> is equal to a change in 529 hydrogen of 0.12 kg m<sup>-2</sup>. The above calculations with respect to biomass variability disregard the 530 fact that fallen leaves still contain hydrogen (which hence is not completely removed from the 531 532 system immediately and therefore should also reduce the expected variability). At our field site 533 65 % of the distance-weighted area surrounding the CRS is covered by deciduous trees (mainly beech and oak), the other 35 % do not experience a significant annual cycle of leaf growth and 534 fall (pine, spruce and grassland). This should further reduce the influence of seasonally variable 535 biomass on the cosmic ray neutron counts (with a potential maximum influence of leaf-out during 536 wet conditions of 0.020 m<sup>3</sup> m<sup>-3</sup> and only 0.012 m<sup>3</sup> m<sup>-3</sup> in dry conditions). In summary, we do not 537 expect a significant impact of seasonally varying above-ground biomass on the measurements of 538 soil water content. Also, we could not find systematic changes in the calibration results connected 539 to the annual cycle of tree foliation/defoliation (i.e. a reduction in counts during summer due to 540 higher hydrogen content in the above-ground biomass). Therefore we deem a correction for 541 variable hydrogen from forest canopy biomass at different times of the year unnecessary. 542

With regard to other varying hydrogen pools we noticed that the influence of interception storage 543 both in the canopy and in the litter layer can potentially have an impact. When both the canopy 544 and the litter layer are wet, the combined hydrogen amount within these two stores can sum up to 545 almost 5 % of the total hydrogen pool equaling a change in volumetric soil water content of 0.067 546  $m^3 m^{-3}$  (Fig. 11). It is not possible to solve this problem by calibrating during conditions of high 547 interception storage since then the soil water content would be underestimated as soon as the 548 549 canopy is dry. Calibration during conditions of dry canopy and litter layer is recommendable because conditions with an empty interception store are generally prevalent and can be much 550 better defined than conditions with a filled interception store. A potential solution to the influence 551 of the variable interception storage filling is the introduction of another neutron count correction 552 using observed, derived or modeled interception storage values (similar to the pressure or the 553 554 water vapor correction).

## 555 5.2. Weighting approaches

556 The fact that the depth-specific weighting (DSW) approach performed better than the simple depth weighting (SDW) is an indication that the depth variations in lattice water, soil organic 557 matter and root biomass content should be explicitly accounted for during the calibration of the 558 CRS. The best performance was achieved with a weighting approach (DDW) that explicitly takes 559 into account both depth-weighting as well as distance weighting of the soil water content (Table 560 7). This suggests that the variation in the footprint diameter needs to be considered during 561 562 individual calibration campaigns. Linear depth-weighting resulted in a better CRS performance than non-linear depth-weighting since the non-linear depth-weighting basically underestimated 563 soil water contents during wet periods (because higher weights of deeper (drier) soil layers were 564 included). This caused both a decrease in the mean soil water content as well as a decrease in the 565 566 variability of the soil water content time series and hence reduced the performance of the CRS. In 567 soils where water content increases with depth the difference between linear and non-linear depth-weighting could be smaller (even negligible), at our field site, however, the decrease of 568 water content with depth apparently favors the use of a linear depth-weighting function. 569

## 570 5.3. Calibration function

The differences in calibration results are likely caused by the fact that the shape of the  $N_0$ -571 calibration function is different at our field site. That means that while being temporally stable 572 the shape of the calibration function is spatially variable - there is no standard curve applicable to 573 574 all sites. At our site the function is less steep than the standard  $N_0$ -calibration function suggested by Desilets et al. (2010), i.e. a similar increase in neutron counts is associated with a smaller 575 decrease in soil moisture. A recalibration of the shape of the curve using all calibration points 576 577 considerably improved the agreement between in situ measurements and CRS measurements of 578 soil moisture. A two-point calibration already proved to be sufficient to define the correct shape 579 of the calibration function given that the soil moisture states at the two calibration times were 580 sufficiently different. In a recent study Iwema et al. (2015) also investigated temporal field 581 sampling strategies for three different calibration methods. They tested combinations of different numbers of random sampling dates and found that using more than six random sampling dates 582 583 did not improve their calibration results much more. However, for the  $N_0$ -calibration method they

found that selecting sampling dates with distinct soil wetness conditions could reduce the 584 585 required number of samplings. In conclusion they also recommended more than one calibration campaign for the  $N_0$ -calibration approach and argued that the shape of the calibration function 586 should not be fixed but kept variable during the calibration process. This is in line with our 587 findings on the shape of the calibration function. The value of the standard No-calibration method 588 becomes apparent when there is only data available from one calibration date. Due to the fixed 589 shape of its calibration function, the general dynamics of the soil water content will still be 590 591 reproduced.

592 We can only speculate about the reasons behind this shape inconsistency of the calibration 593 function for our site since we did not do any theoretical neutron modeling. To our knowledge we are dealing with the lowest number of counts of all published studies (average  $N_0 = 878$  counts h 594 <sup>1</sup>, Table 4). Although the calibration function was theoretically developed for all environments it 595 596 has not yet been tested sufficiently in such low-count, forested environments. Moreover, due to the low neutron count the uncertainty in the determination of soil water content during calibration 597 has a much higher influence on the calibration results than in high-count environments. Bogena et 598 al. (2013) pointed out another complicating factor that is present in forested environments – the 599 litter layer. They showed that at their sites ( $N_0$ : 913 to 1397 counts h<sup>-1</sup>) the model-derived water 600 content within the litter layer (under spruce) was subject to much higher variability than the water 601 602 content in the underlying soil. During wet conditions the water within the litter layer contained 36 % of the hydrogen mass within the footprint of the CRS while during dry conditions it contained 603 only 10 % of the hydrogen mass. This leads to an increase in the variability of the neutron counts 604 and can thus cause an overestimation of soil water content during wet conditions. Although the 605 water within the litter layer at our site accounts for a much smaller fraction of the total hydrogen 606 pool (up to 3 %) it can still have an influence on the neutron counts and the calibration results. 607 608 The occurrence of canopy interception would have the same variability-increasing effect on the CRS signal, although it is expected to be significantly smaller than the influence of the litter 609 layer. Baatz et al. (2014) working also in a low-count environment ( $N_0$ : 936 to 1242 counts h<sup>-1</sup>) 610 with land use ranging from grassland to agriculture to forest compared the standard  $N_0$ -calibration 611 method to another parameterization calibration method developed by Shuttleworth et al. (2013) 612 (the COSMIC operator, a model of neutron intensity used in data assimilation schemes) and 613 found that the former interpreted dry periods drier and wet periods wetter - which is in 614

**Kommentar [A6]:** Ref3: this is not a calibration method, but a model of neutron intensity that can be used in data assimilation schemes - please clarify this in text.

accordance to our findings that suggest that the standard N<sub>0</sub>-calibration function is too steep. Lv 615 616 et al. (2014), in a study at a mixed-forest/grassland site also recommended more than one calibration. They operated in a high-count environment in Utah ( $N_0 = 2189$  counts h<sup>-1</sup>) and 617 618 attributed the different shape of their calibration function to binary soil moisture patterns at their site where the grassland soils were much drier than the forest soils under wet conditions but just 619 as dry under dry conditions. Our field site is subject to similar spatial variability since it is also 620 comprised of multiple areas with non-uniform soil water content (mean values of soil water 621 622 contents differ between different forest stands). Following the argumentation of Lv et al. (2014), 623 the fact that distance weighting improved our results can be regarded as an indication that non-624 homogeneous soil moisture conditions indeed lead to changes in the shape of the calibration function. At our site, distance weighting reduced the spatial variability within the footprint of the 625 626 sensor since it assigned higher weights to the closest sampling sites which were all located in the 627 homogenous and relatively wet beech forest, while the influence of the drier soils under the coniferous trees was reduced. 628

If it was possible to fully correct for all factors that influence footprint size, depth-weighting and 629 630 neutron count, a one-time calibration of the CRS would be sufficient. However, the abundance of different hydrogen pools and the uncertainties in the sensing depth estimation will always lead to 631 uncertainties in the calibration process. Therefore we argue that for the use of the CRS as a 632 633 simple tool to measure soil water content at intermediate scales, the efforts of measuring all necessary parameters are not justified. As shown by Iwema et al. (2015) and by the results of this 634 study, this issue can be dealt with by using site-specific calibration parameters estimated from in 635 situ samples taken during dry and wet conditions. Hence, we recommend a two-point calibration 636 that - although being empirical in nature - inherently incorporates many of the required 637 corrections. 638

639

# 640 6. Conclusion

641 Our results suggest that a one-time calibration of the CRS using the available neutron count 642 corrections and weighting approaches is not sufficient at our field site. This is mainly due to the 643 fact that the shape of the standard  $N_0$ -calibration function is not able to reproduce the dynamics in

soil water content we observed with our network of distributed in situ TDT sensors. Several 644 645 factors could cause this discrepancy, amongst them the presence of a litter layer and spatially heterogeneous soil moisture conditions within the sensor footprint. After calibrating the CRS 10 646 times in a mixed forest in north eastern Germany we found that a two-point calibration already 647 considerably improved the agreement between soil water content derived from in situ TDT 648 measurements and from the CRS, given significantly different moisture conditions during the two 649 calibration periods/campaigns (for a detailed explanation on the procedure see Appendix A). We 650 found that the explicit consideration of depth-specific values of soil organic matter and root 651 652 biomass improved the calibration results while seasonal changes in above-ground biomass in the 653 forest were found to be negligible. While there is no doubt that further investigations of factors that influence the neutron signal are necessary and useful, it is also apparent that it becomes 654 655 increasingly difficult to distinguish between the effects of the individual correction factors and 656 the uncertainty caused by all the corrections. Therefore our goal was to use empirical data to test available methods and combinations thereof and to provide a guideline on how to easily and 657 comprehensively calibrate a CRS in various environments using these methods. Looking beyond 658 that objective, site intercomparison studies along gradients from high to low-count environments 659 and/or from locations with varying litter layers could give rise to the development of simple 660 corrections to the shape of the  $N_0$ -calibration function. 661

When measuring soil water content with a CRS it is important to note that over time the measurements are hardly ever representative of the exact same soil segment around and below the sensor (Köhli et al, 2015). With the footprint shrinking and expanding and the effective measurement depth in the soil decreasing and increasing we have to be careful when interpreting and using our results. If we keep that in mind, however, this new technology will indeed be able to bridge the gap between point in-situ and areal remote sensing soil moisture measurements and thus provide a valuable tool for the advancement of hydrologic understanding.

669

670 Appendix A: <u>Proposed</u>Best <u>method</u>practice for calibration in low-count forest 671 environments Kommentar [A7]: Ref3: I am not sure if this is best practice. It is yours, but to be best it should be confirmed by others. I suggest deleting this appendix. Or, at the very least, present it as a proposal for consideration by users.

Kommentar [A8]: Reply: You are right in that we should not call it 'best practice'. This would indeed be overconfident. Therefore we changed the name to 'Proposed practice for calibration...' We would, however, like to keep the Appendix in the manuscript since it provides the sequence of necessary steps that first-time users can follow when they set up and calibrate the instrument. When we started we would have liked to find such a condensed and structured compilation.

- 672 We provide an Excel file as a supplement to perform the calculations described in the following
- 673 step-by-step instructions.
- Set up (or use) a weather station that monitors air temperature and relative humidity close to
   the CRS.
- 676 2. Set up the CRS in a location where the conditions within a radius of at least 30 m around
  677 the sensor are relatively homogeneous (similar soils, tree species, expected soil moisture
  678 conditions).
- Switch on the CRS and come back later for calibration (or set it up before 6 a.m. and start calibrating on the same day). You should at least have 12 hours of CRS data for one calibration. Do not switch it off after the calibration, let it record continuously.
- 4. Choose a day with very dry or very wet soil moisture conditions for the first calibration
  campaign and wait for the opposite conditions for your second calibration (this might take a
  full year to achieve, but you will not lose any data, you will just not be able to accurately
  convert the data immediately).
- 5. Choose days without rain or snow for your calibrations, litter and canopy should be dry.
- 6. Take 108 soil samples from 18 locations (six directions, three distances) and six depths (0-30 cm). For equal distance weights choose distances according to Köhli et al. (2015) (~1, ~33 and ~140 m).
- 690 7. Weigh the samples the same day you take them, let them oven-dry for 24 h at 105°C and 691 weigh them again to determine the volumetric water content ( $\theta$ ) and the bulk density ( $\rho_{bd}$ ).
- 692 8. Create six bulk samples from the six different soil depths (2 g from each of the 18 locations693 suffices for each soil depth).
- 694 9. Determine the combined soil organic matter (SOM) and root biomass ( $B_R$ ) content of the 695 six bulk samples by weighing them (after regular oven-drying at 105°C) and then heating 696 them to a temperature of 400°C for 24 h before weighing them again. Convert SOM and  $B_R$ 697 to water equivalents by multiplying the weight by 0.556.
- 698 Caution: In clay-rich soils this method tends to overestimate soil organic matter content
  699 because some of the lattice water is removed already at temperatures around 400°C
  700 (Howard and Howard, 1990).

701	10.	Determine the lattice water $(W_L)$ content of the six bulk samples by weighing them (after
702		SOM and $B_R$ extraction at 400°C) and then heating them to a temperature of 1000°C for 24
703		h before weighing them again.

- Caution: Carbonate-rich soils experience thermal breakdown of carbonates at temperatures
   above 430°C (Ben-Dor and Banin, 1989).
- Determine the water equivalent of the average hydrogen content of belowground hydrogen
   pools (H<sub>p</sub>) for each soil depth.

708 Equation (8).

709 12. Apply a linear weighting function to your gravimetrically determined  $H_p$  measurements 710 accounting for the change in the effective measurement depth z\* of the sensor and retrieve a weighted average of H<sub>p</sub> within the footprint of the CRS by iteration. Start out by computing 711 712 the effective measurement depth z\* corresponding to your gravimetrically determined 713 values of H<sub>p</sub> and p<sub>bd</sub> averaged over the entire 30 cm. Then apply the weights for the different soil depths z and update the values. Recalculate the effective measurement depth 714 and continue this procedure until all values stabilize. Do this for each 715 z\* sampling/calibration distance (~1, ~33 and ~140 m) separately. 716

717 Equations (5), (6) and (9).

- Apply an additional distance-weight to the depth-weighted volumetric water contents from
  the different locations in order to account for variations in the footprint size. Also do this
  iteratively adjusting H<sub>p</sub> and the distance weights until both become stable.
- Equations are conveniently provided as a supplement by Köhli et al. (2015) in the form ofan Excel file.
- 14. Use the depth-and-distance weights to compute weighted values of soil water content ( $\theta$ ), bulk density ( $\rho_{bd}$ ), lattice water ( $W_L$ ), soil organic matter and root biomass water equivalent (SOM+B<sub>R</sub>).
- 15. Average raw neutron counts (N<sub>raw</sub>) from the moderated sensor (measuring fast neutrons)
  over 12 h with a moving window.
- Retrieve data from the neutron monitor close to your location in order to correct for the varying intensity of incoming neutrons (you may have to correct this data and fill gaps).
- 17. Using the entire time series for the period where cosmic-ray data is available determine average atmospheric pressure (P<sub>0</sub>), average incoming neutron intensity (N<sub>avg</sub>) and average absolute humidity ( $p_{v0}^{ref}$ ).

735	19.	Correct raw neutron counts for incoming neutron intensity variations (N <sub>pi</sub> ).
736		Equation (2).
737	20.	Correct raw neutron counts for absolute humidity variations (N <sub>pih</sub> ).
738		Equation (3).
739	21.	Fit a function through the two calibration points altering $N_0$ , $a_0$ , $a_1$ and $a_2$ (e.g. using
740		Microsoft Excel solver). When doing this, use average values of the two calibration
741		campaigns for bulk density ( $\rho_{bd}),$ lattice water (W_L), soil organic matter and root biomass
742		water equivalent (SOM+B <sub>R</sub> ).
743	22.	Plot the $N_{\text{pih}}\xspace$ of both calibrations against the gravimetrically measured, distance- and depth-
744		weighted volumetric soil water content ( $\theta$ ).

18. Correct raw neutron counts for atmospheric pressure variations (N<sub>p</sub>).

745 23. Use best fit parameters to convert time series of  $N_{pih}$  to volumetric soil water content.

746

733 734

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Equation (1).

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893 Table 1. Fractions of different tree stands in percent within the footprint of the CRS. The total 894 represents a distance weighted average with an exponential decay towards more distant areas

## (approximating the exponential distance-weighting from Zreda et al. (2008)). 895

	Radius 0-50 m	Radius 50-150 m	Radius 150-300 m	Total
Beech	85.2	32.8	48.7	55.5
Pine	3.0	26.3	17.6	15.6
Spruce	5.8	20.9	11.1	12.6
Oak	0.0	10.3	12.5	7.6
Open (grass)	6.0	9.7	3.9	6.5
Larch	0.0	0.0	5.5	1.8
Birch	0.0	0.0	0.7	0.2

896

897	Table 2. Overview of the four weighting approaches for other than soil moisture effects on the
898	CRS signal.

Approach	1 SDW	2 DSW	3 DDW	4 DDWnl
consideration of depth-specific $W_L$ and SOM+B <sub>R</sub>	no	yes	yes	yes
distance depth-weighting	no	no	yes	yes
non-linear depth-weighting	no	no	no	yes

Table 3. Example of depth weighting (DSW) for an effective measurement depth of  $z^* = 22.1$  cm, a = 0.0903 and b = 1. Calibration campaign date 21 November 2014 (F4). Note the difference in

specific weights if only soil water content  $\theta$  is considered (wt(z, $\theta$ )) or if  $W_L$  and  $SOM + B_R$  is also

903 considered (wt(z, $H_p$ )).

Layer (cm)	$\theta$ (m <sup>3</sup> m <sup>-3</sup> )	$W_{L} (m^{3} m^{-3})$	$\frac{\text{SOM+B}_{R}}{(\text{m}^{3}\text{ m}^{-3})}$	$H_{p}(m^{3}m^{-3})$	ρ <sub>bd</sub> (g cm <sup>-3</sup> )
0-5	0.187	0.002	0.034	0.223	0.669
5-10	0.136	0.004	0.024	0.163	1.143
10-15	0.117	0.004	0.019	0.140	1.217
15-20	0.109	0.004	0.015	0.129	1.256
20-25	0.106	0.005	0.013	0.124	1.359
25-30	0.100	0.005	0.012	0.118	1.431

904

z (cm)	$wt(z, \theta)$	$\int_{\mathbf{z}}^{\mathbf{z}+5} \mathbf{wt}(\mathbf{z}, \mathbf{\theta})$	$\operatorname{wt}(\mathbf{z}, H_p)$	$\int_{z}^{z+5} \operatorname{wt}(z, H_p)$
0	0.079	0.356	0.090	0.401
5	0.063	0.278	0.070	0.299
10	0.048	0.200	0.050	0.197
15	0.032	0.122	0.029	0.095
20	0.017	0.044	0.009	0.009
25	0.001	0.000	0.000	0.000
		Σ=1.00		Σ=1.00

Table 4. Atmospheric and soil parameters as well as neutron counts for the 10 calibrations. 906 907 Atmospheric pressure P, absolute humidity  $p_{v0}$ , raw neutron count  $N_{raw}$ , pressure corrected 908 neutron count N<sub>p</sub>, pressure and incoming radiation corrected neutron count N<sub>pi</sub>, pressure, incoming radiation and water vapor corrected neutron count  $N_{pih}$ , calibration neutron count  $N_0$ , 909 910 incoming radiation from the neutron monitor  $N_{\rm nm}$ , average soil moisture of the top 30 cm  $\theta_{\rm 30cm}$ , depth-weighted soil moisture  $\theta_{depthW}$ , depth-weighted sum of volumetric lattice water content, soil 911 organic matter and root biomass water equivalent  $(W_L+SOM+B_R)_{depthW}$ , depth-weighted water 912 913 equivalent of belowground hydrogen pools  $(H_p)_{depthW}$ , depth-weighted bulk density  $(\rho_{bd})_{depthW}$  and 914 average volumetric soil water content  $\theta_{mod}$  of the resulting time series using the N<sub>0</sub>-calibration 915 function with standard parameters. Mean ( $\mu$ ) and standard deviation ( $\sigma$ ) values of the 10 916 calibration campaigns are given in the two bottom lines.

Calibration	P (hPa)	p <sub>v0</sub> (g m <sup>-3</sup> )	N <sub>raw</sub> (counts h <sup>-</sup> <sup>1</sup> )	N <sub>p</sub> (counts h <sup>-</sup> <sup>1</sup> )	$N_{pi}$ (counts h <sup>-1</sup> )	$N_{pih}$ (counts h <sup>-1</sup> )	$N_0$ (counts h <sup>-1</sup> )
Winter	984.0	5.7	606.2	514.9	518.8	509.4	872.4
Spring1	999.3	8.6	549.2	523.0	527.5	526.2	868.7
Spring2	1021.0	4.9	491.1	550.6	542.8	530.5	871.1
Spring3	1002.9	9.6	544.7	533.1	539.9	541.5	869.2
Spring4	1019.0	8.0	503.4	556.0	549.4	546.1	879.0
Summer	1008.7	14.0	613.3	626.6	623.8	640.5	858.2
Fall1	998.7	11.5	624.7	592.4	593.8	601.5	909.5
Fall2	1014.1	7.8	509.3	542.1	546.7	542.8	876.2
Fall3	990.3	8.5	630.4	561.4	580.4	578.5	892.8
Fall4	1016.7	6.6	544.4	591.0	577.7	569.9	885.7
μ	1005.5	8.5	561.7	559.1	560.1	558.7	878.3
σ	11.9	2.6	50.2	33.1	31.1	37.5	13.8

Calibration	N <sub>nm</sub> (count s h <sup>-1</sup> )	$\begin{array}{c} \theta_{30cm} \\ (m^3 m^3 m^3) \end{array}$	$\theta_{depthW}$ (m <sup>3</sup> m <sup>-</sup> <sup>3</sup> )	$\begin{array}{c} (W_L + SOM \\ + B_R)_{depthW} \\ (m^3 \ m^{-3}) \end{array}$	$(\mathbf{H}_{p})_{depthW}$ $(\mathbf{m}^{3} \mathbf{m}^{-3})$	(ρ <sub>bd</sub> ) <sub>depthW</sub> (g cm <sup>-3</sup> )	$(\mathbf{m^3 m^{-3}})$
Winter	325.8	0.163	0.228	0.0343	0.262	0.985	0.141
Spring1	325.5	0.153	0.200	0.0340	0.234	1.013	0.143
Spring2	333.0	0.150	0.185	0.0311	0.216	0.955	0.137
Spring3	324.1	0.140	0.175	0.0324	0.207	1.000	0.143
Spring4	332.2	0.139	0.170	0.0302	0.200	0.957	0.145
Summer	329.8	0.073	0.080	0.0278	0.108	1.074	0.151
							20

Fall1	327.4	0.112	0.137	0.0299	0.167	1.016	0.182
Fall2	325.5	0.140	0.174	0.0310	0.205	0.970	0.144
Fall3	317.5	0.119	0.149	0.0316	0.181	1.018	0.166
Fall4	335.8	0.126	0.150	0.0293	0.179	0.981	0.155
μ	327.7	0.131	0.165	0.0312	0.196	0.997	0.151
σ	5.0	0.024	0.038	0.0019	0.039	0.034	0.013

919 Table 5. Means ( $\mu$ ) and standard deviations ( $\sigma$ ) of calibration parameter  $N_0$  and means ( $\mu$ ) and 920 standard deviations ( $\sigma$ ) of resulting time series of volumetric soil water content  $\theta_{mod}$  for the four 921 weighting approaches with 10 calibration campaigns each.

Approach	$(N_0)_{\mu}$ (counts h <sup>-1</sup> )	$(N_0)_{\sigma}$ (counts h <sup>-1</sup> )	$(\theta_{mod})_{\mu} (m^3 m^{-3})$	$(\theta_{mod})_{\sigma} (m^3 m^{-3})$
1 SDW	855.0	17.3	0.158	0.015
2 DSW	878.3	13.8	0.151	0.013
3 DDW	841.9	13.7	0.139	0.012
4 DDWnl	828.1	13.3	0.134	0.012

923 Table 6. Modified calibration parameters for the four weighting approaches.

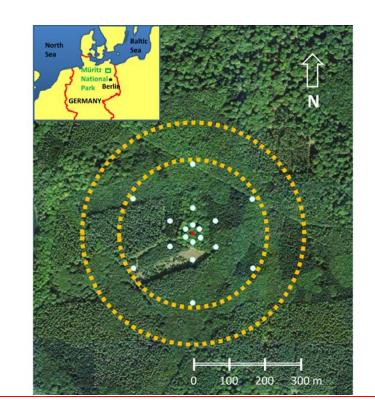
	$N_0$	$\mathbf{a}_0$	$\mathbf{a}_1$	$\mathbf{a}_2$
1 SDW	926.3	0.203	0.109	0.238
2 DSW	1007.8	0.203	0.114	0.267
3 DDW	810.7	0.326	0.001	0.310
4 DDWnl	779.3	0.314	0.001	0.285

Table 7. Performance measures for the four weighting approaches – comparison of modified calibration (mdf) with standard calibration (stan). KGE' is the modified Kling-Gupta efficiency,  $\beta$  is the bias ratio and  $\gamma$  is the variability ratio. (KGE')<sub>µ</sub> and (KGE')<sub>σ</sub> represent the mean and standard deviation of the KGE' values of the 10 individual single-point standard calibrations.

	KGE'			(KGE'	(KGE'		
	mdf	β mdf	γ mdf	stan) <sub>µ</sub>	$stan)_{\sigma}$	$(\beta \ stan)_{\mu}$	$(\gamma \ stan)_{\mu}$
1 SDW	0.830	0.849	0.986	0.675	0.045	1.120	1.258
2 DSW	0.880	0.915	0.964	0.727	0.035	1.032	1.231
3 DDW	0.891	1.076	0.986	0.712	0.081	0.878	1.237
4 DDWnl	0.833	1.148	1.011	0.681	0.096	0.818	1.244

Table 8. Hydrogen pools (in kg hydrogen per m<sup>2</sup>) in the CRS footprint for different moisture
conditions (wet: 0.29 m<sup>3</sup> m<sup>-3</sup>, full canopy and litter storage; intermediate: 0.17 m<sup>3</sup> m<sup>-3</sup>, dry canopy
and moist litter storage; dry: 0.05 m<sup>3</sup> m<sup>-3</sup>). Above-ground biomass is split into a static part (AGB
wet static) comprising stem, branches and dry litter and a variable part (AGB wet variable) that
represents leaves.

Hydrogen Pool	Wet (kg m <sup>-2</sup> )	Intermediate (kg m <sup>-2</sup> )	Dry (kg m <sup>-2</sup> )
AGB wet static	5.24	5.24	5.24
AGB wet variable	0.22	0.22	0.22
SOM+R <sub>B</sub>	0.36	0.44	0.66
Lattice water	0.05	0.07	0.15
Pore water	4.12	3.26	1.77
Litter water	0.31	0.11	0.00
Interception	0.17	0.00	0.00
Total	10.47	9.35	8.04



944

Figure 1. Soil sampling locations for calibration (whiteblue dots) and forest vegetation around the
CRS (red dot in the center). The TDT soil moisture sensors are located in close vicinity to the
sampling locations. The larger yellow circle approximates the footprint of the CRS as it was
assumed when sampling took place (diameter approximately 300 m). The smaller yellow circle
approximates the footprint of the CRS according to newer modeling results by Köhli et al. (2015)
(diameter approximately 200 m). Inset: Field site location in Müritz National Park in northeastern Germany.

Kommentar [A11]: Ref1: The blue dots are difficult to discern

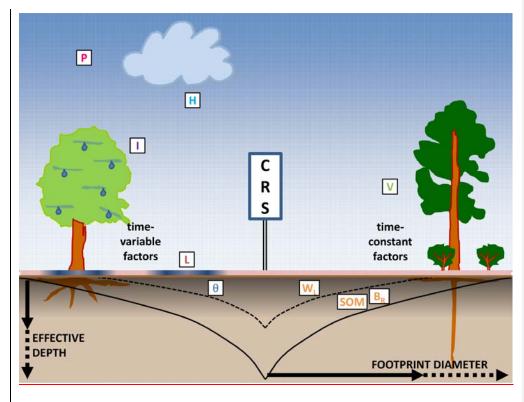
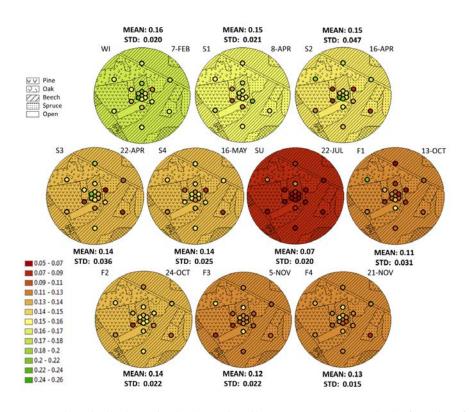


Figure 2. Simplified representation of factors influencing the raw neutron count  $(N_{nav})$  and the 946 947 measurement support volume of the CRS in terms of effective measurement depth and footprint. Temporally variable factors are shown on the left: barometric pressure (P), canopy interception 948 949 (I), air humidity (H) and litter layer interception (L). Temporally constant factors (for our study 950 site) are shown on the right: vegetation above and below the sensor (V), soil organic matter (SOM), root biomass (B<sub>R</sub>) and lattice water (W<sub>L</sub>). All these factors need to be accounted for in 951 order to isolate the soil water content signal ( $\theta$ ). The time-variable factors require permanent 952 monitoring and dynamic correction, the influence of the constant factors is taken into account 953 during calibration. The combination of the-time-variable and time-constant factors leads to a 954 955 reduction of the maximum effective depth and footprint diameter (solid black line) and creates a site specific temporally variable effective measurement depth and footprint diameter (dashed 956 black line). 957

Kommentar [A12]: Ref1: The modified schematic shown in this figure is still confusing. Why should the factors influencing the cosmic-ray intensity a ground level be symbolized a rays of different length? I find this irritating and not helpful for the understanding of the involved processes. In addition, the presented sensing depth boundaries are too numerous be discernible and the distribution is not correct. A better representation can be found in Köhli et al., 2015. Thus, in my opinion the figure should be omitted.

Kommentar [A13]: Reply: We modified the figure to address your concerns. We removed the rays of different length and instead used gradually less intense background color to represent the decreasing number of fast neutrons due to the various factors. We removed all depth boundaries only keeping the maximum extent and one example of reduced depth and footprint. We also modified the shape of the depth boundary so that it resembles better what Köhli et al. (2015) describe.

Kommentar [A14]: Ref3: support volume may be a better term here



959

Figure 3. Gravimetrically determined volumetric soil water content patterns in the footprint of the CRS for the 10 calibration dates. The colored dots indicate the unweighted average value from 0 to 30 cm at the 18 calibration locations. Background colors represent the unweighted average value of all 108 soil samples. Different forest stands (pine, beech, oak, spruce) are indicated by the patterned background.

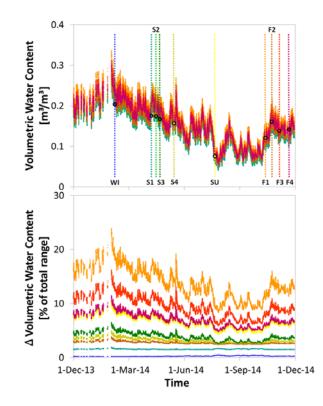
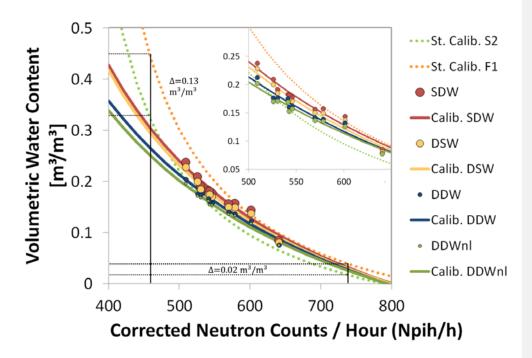
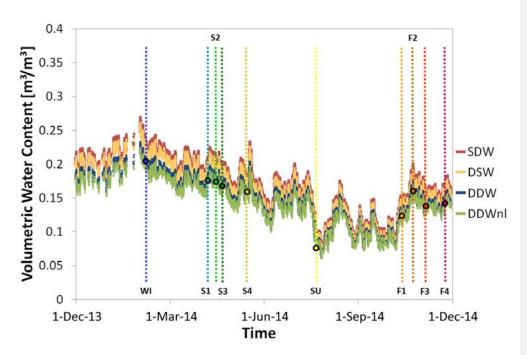


Figure 4. Upper panel: volumetric water content derived from CRS data for each of the 10 calibration dates separately (vertical lines indicate calibration dates, colors correspond to time series colors). Filled circles represent the weighted volumetric water content at the time of calibration (according to DDW). Lower panel: differences in water content between calibration S1 and all other calibrations expressed as a percentage of the total possible range of average soil water content – ranging from 0.04 m<sup>3</sup> m<sup>-3</sup> to 0.34 m<sup>3</sup> m<sup>-3</sup>at our field site (color coding corresponds to calibration dates in the upper panel).



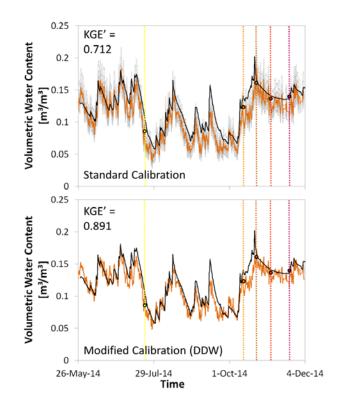
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976 Figure 5. Modified calibration functions (solid lines) for the four different weighting approaches (simple depth-weighting SDW, depth-specific weighting DSW, distance-depth-weighting DDW, 977 distance-depth-weighting, non-linear DDWnl), each one derived from 10 calibration points 978 979 (circles). Calibration points are better captured by flatter calibration functions (solid lines) with modified calibration parameters than by any of the standard calibration functions (dotted lines) 980 based on a single calibration data set only (days S2 and F1 as an example). Black lines illustrate 981 982 that differences in soil moisture between the results of individual calibrations are larger when soil moisture is high. The inset magnifies the area around the calibration points. 983



985

Figure 6. Time series of volumetric water content derived with modified calibration functions using parameters based on the four calibration approaches: simple depth-weighting (SDW), depth-specific weighting (DSW), distance-depth-weighting (DDW) and distance-depthweighting, non-linear (DDWnl). Filled circles represent the weighted average of volumetric water content obtained from soil cores at the time of calibration (weighting according to DDW).



993 Figure 7. Average volumetric water content derived from TDT point measurements (black line) and CRS measurements (orange line) using different calibration functions. Upper panel: the 994 995 orange line is an average of the volumetric water content derived from the 10 calibration 996 campaigns of the CRS using the standard  $N_0$ -calibration function from Desilets et al. (2010) applying the DDW approach. Grey dotted lines are results for 10 individual calibration 997 campaigns (KGE' values range from 0.579 to 0.834). Lower panel: the orange line is the 998 volumetric water content derived from the calibration function with modified calibration 999 parameters applying the DDW weighting approach based on all 10 calibration dates. The colored 1000 1001 vertical lines mark the days of the last five calibration campaigns.

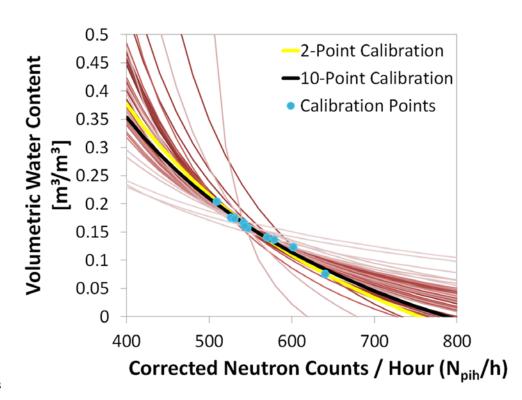
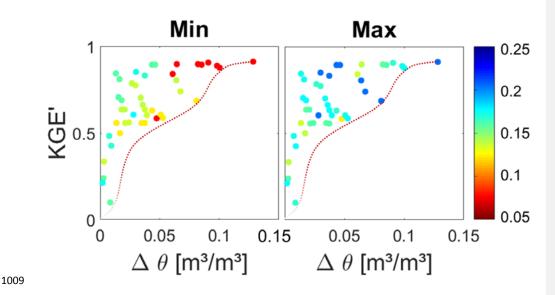




Figure 8. Best-fit  $N_0$ -calibration functions (red-brown colored lines) for all combinations of twopoint calibrations (blue dots). Best-fit  $N_0$ -calibration function for 10-point calibration (black line). Best-fit two-point  $N_0$ -calibration function derived from calibration points with highest and lowest volumetric water content (yellow line).



1010 Figure 9. Performance of CRS soil water content data derived from two-point calibrations in 1011 relation to difference between soil moisture states ( $\Delta \theta$ ) at the two calibration dates. The color bar 1012 indicates volumetric soil water content. Left panel: points are colored according to the soil water 1013 content of the drier calibration date. Right panel: points are colored according to the soil water 1014 content of the wetter calibration date. Dashed lines indicate that soil moisture differences of less 1015 than 0.1 m<sup>3</sup> m<sup>-3</sup> can produce  $N_0$ -calibration curves with sub-optimal conversions of neutron 1016 counts to volumetric soil water content.

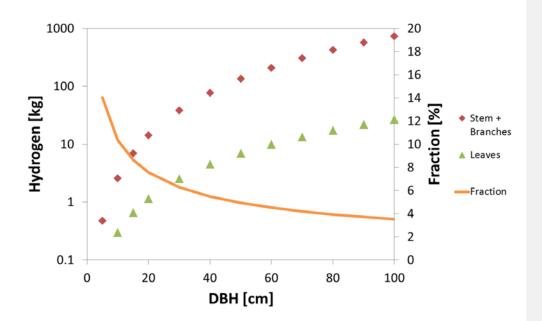


Figure 10. Mass of hydrogen in individual beech trees in stem and branches (red diamonds) and
leaves (green triangles) in relation to diameter at breast height (DBH). Fraction of leaf hydrogen
mass to total aboveground tree hydrogen mass (orange line).

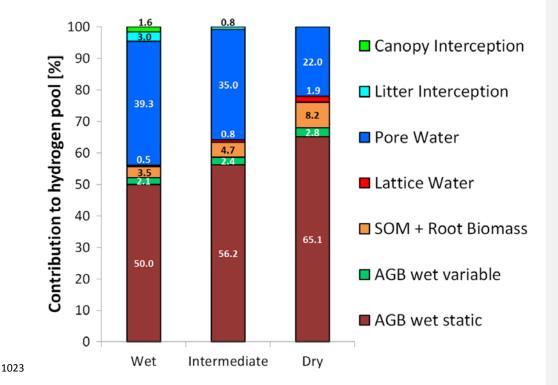
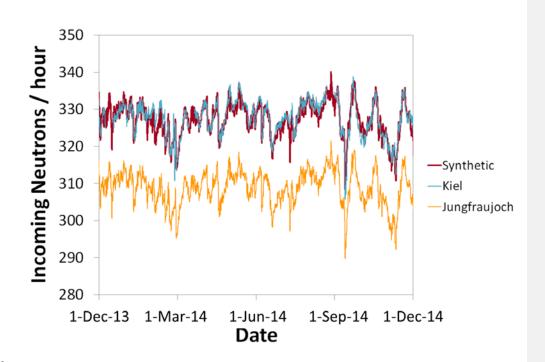
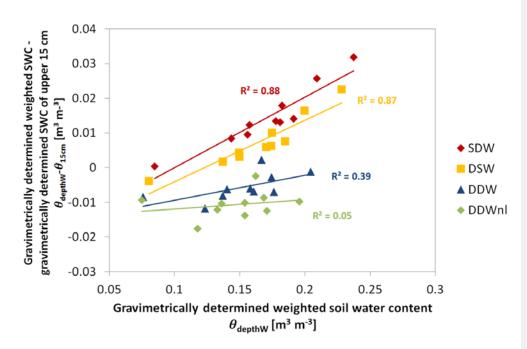


Figure 11: Varying hydrogen pools in the beech forest surrounding the CRS for three different site conditions. AGB (above-ground biomass) wet variable represents hydrogen contained in deciduous leaves (both in the biomass and in the leaf water). AGB wet static comprises hydrogen contained in biomass and water of tree stems and branches as well as in biomass of the litter layer.



1031 Figure S1. Incoming neutron flux from the neutron monitors in Kiel, Germany and Jungfraujoch,

Switzerland and synthetic continuous time series of incoming neutron flux combined from these two and used for the corrections in this study. 



1035

Figure S2. Comparison of depth-(and distance-) weighted averages of gravimetrically determined soil water content with unweighted gravimetrically determined soil water content of the upper 15 cm of the soil. The first two weighting approaches overestimate soil water content in the upper 15 cm especially at high soil water contents. The last two approaches have only a slight negative offset and no significant relationship with wetness conditions.