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Evaluating soil moisture simulations from a national-scale gridded hydrological model over Great Britain

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ABSTRACT

Study Region: The study covers sites across Great Britain.
Study Focus: Soil moisture information is important for a range of applications including flood and drought monitoring, seasonal hydrological forecasting, and agricultural management. However, spatially distributed soil moisture estimates for sub-surface soils are scarce despite their importance. The Grid-to-Grid hydrological model (G2G) was primarily developed to simulate river flows at a national scale, but can also output simulated depth-integrated soil moisture on a 1 km grid. Here, we evaluate G2G soil moisture simulations against in situ neutron probe (NP) observations at 85 sites across Great Britain, to evaluate whether modelled soil moisture outputs have value and to identify areas for improvement.
New Hydrological Insights for the Region:: Despite large uncertainties in observed soil moisture within a site, there was a good temporal correlation between observed and modelled soil moisture, with Pearson correlation values exceeding 0.7 for 77% of sites. However, the model tended to under-predict soil moisture values (median bias of −12 cm/m) and over-predict variation (median standard deviation error of 2 cm/m). Model agreement with observations was generally better for areas with deep or mid-depth mineral soils and worst in areas of peat. Based on this evaluation against NP observations, we demonstrate that G2G soil moisture is a useful resource for estimating relative wetness of the soil, but not necessarily the soil moisture content values themselves.

1. Introduction

Soil moisture content, here defined as the volume of water contained within the unsaturated soil zone, plays a key role in the hydrological cycle (Seneviratne et al., 2010). It regulates the partitioning of rainfall into runoff, evapotranspiration and groundwater storage, and is the main water source for agriculture and natural vegetation (Robock, 2003). As such, soil moisture is a key variable for understanding and predicting river flows, floods and droughts (Chifflard et al., 2018; Sheffield et al., 2014; Wanders et al., 2014; Xu et al., 2020). Studies have shown that most floods in Great Britain (GB) are a result of high antecedent soil moisture combined with heavy rainfall, highlighting the importance of soil moisture in flood generation processes (Berghuijs et al., 2019; Stein et al., 2020). An understanding of soil moisture throughout the soil-column is therefore vitally important for hydrological modelling, and soil moisture observations/simulations can help predict developing flood or drought events.

Most hydrological models include a representation of soil moisture storage or soil moisture deficit, although this can vary widely

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between models from a simple lumped catchment-average soil moisture store to a fully distributed set of stores that vary by depth (e.g. Clark et al., 2008; Coxon et al., 2019; Lindström et al., 1997). An accurate representation of soil moisture in hydrological models is important for multiple reasons. Firstly, soil moisture plays an important role in runoff generation (Bronstert and Bárdossy, 1999; Western et al., 2002), and therefore it needs to be correctly captured even if a model is only required to output simulated flows. This is particularly important in applications where a model is used to simulate change (e.g. climate change, land-use changes) for which we need to be sure that hydrological processes are simulated correctly. Second, simulated soil moisture outputs can also be useful in and of themselves. There is a need for soil moisture products, for example as inputs to crop models, ecosystem models, or drought and flood monitoring systems, but in situ observations are limited in time and space (Xia et al., 2014). Model simulations can provide data where observations are unavailable, including predictions of soil moisture under catchment change or into the future.

Hydrological models are usually evaluated against river flows, as this is the primary variable of interest (Bell et al., 2017; Knoben et al., 2020; Lane et al., 2019; Nicolle et al., 2014). However, evaluations of model outputs against soil moisture observations are also informative, as it does not always follow that a good simulation for river flows is correctly capturing soil moisture dynamics. Evaluating model soil moisture is therefore useful as a form of model internal validation (Fawcett et al., 1995) and essential if the model soil moisture values are going to be provided as outputs. Some previous studies have evaluated model simulated soil moisture (Albergel et al., 2010; Peng et al., 2021; Tso et al., 2023; Xia et al., 2014). For example, Xia et al., (2014) evaluated the soil moisture outputs of four land-surface models (including SAC and VIC which were derived from hydrological models) across the United States of America. They learned that while all models could capture wet and dry events, there were large biases between modelled and observed soil moisture values. Similarly, Peng et al., (2021) evaluated soil moisture simulations from the JULES land-surface model against soil moisture observations from the COSMOS-UK network and found that whilst JULES estimates generally correlated well with observed soil moisture, there were high errors for stations with organic soils. These studies demonstrate the importance of comprehensively evaluating soil moisture simulations, to inform users of their suitability for a range of applications and to guide model improvement.

Soil moisture observations are available from different methods, including in situ observations or satellite data, each with their own merits and disadvantages (Babaeian et al., 2019; Brocca et al., 2011; Evans et al., 2016). Satellite measurements can give soil moisture estimates covering large areas, but are limited to the soil surface (~0–5 cm) and generally have low accuracy (Al-Sharafany, 2021; Dobriyal et al., 2012). On the other hand, ground-based techniques are limited in spatial scale, only providing small-scale measurements which may not capture the heterogeneity of soil moisture patterns, but tend to be more accurate (Dobriyal et al., 2012). Among the ground based techniques, cosmic ray neutron sensors can measure over larger areas (field-scale, up to 200 m radius), but are limited to surface soil moisture only (Cooper et al., 2021). Other methods, such as the use of neutron probes, can measure soil moisture at greater depths, but measurements cover smaller areas (point-scale, around a 30 cm radius) (Bell et al., 2022). Both satellite-based and in situ soil moisture measurements can have large uncertainties (Baroni et al., 2017; McMillan et al., 2018).

A newly collated set of soil moisture observations, the UK Soil Moisture Databank, has recently been made available, driven by the growing requirement for long-term, geographically distributed data against which to assess the performance of national-scale hydrological models (Bell et al., 2022). This dataset collates in situ neutron probe (NP) measurements of soil moisture taken at numerous sites across GB since the late 1960 s, including an historical dataset of neutron-probe observations previously thought lost (Gardner, 1981). Compared to other available datasets for GB, the UK Soil Moisture Databank has several key advantages for use in the evaluation of a national-scale hydrological model: 1) neutron probes yield reasonably accurate measurements of soil moisture, 2) the dataset includes measurements at depths of up to several metres, and 3) some measurements span a long time period (over 15 years).

The Grid-to-Grid (G2G) hydrological model was developed with the aim of simulating river flows, but it also has the capability to output estimates of soil moisture (Bell et al., 2009). It has been widely applied in hydrological applications across the UK including for floods (Bell et al., 2009; Kay et al., 2021a; Lane and Kay, 2021), droughts (Rudd et al., 2019), and seasonal river flow forecasts (Bell et al., 2017). More recently there has been interest in G2G soil moisture outputs, and the value these could have in seasonal forecasting and climate change impact analyses (Bell et al., 2018; Kay et al., 2022a; UKCEH, 2023a). However, so far there has been no evaluation of G2G against soil moisture observations, only evaluations of model outputs compared to observed river flows (Bell et al., 2009, 2007a; Price et al., 2012; Rudd et al., 2017) and a modelled soil moisture product (Kay et al., 2022a). This raises the question of whether the hydrological model that produces reasonable estimates of river flows also correctly captures patterns of soil moisture.

Here, we evaluate gridded soil moisture outputs from G2G against NP soil moisture observations from the UK Soil Moisture Databank. The recent release of the UK Soil Moisture Databank has made such an evaluation possible for the first time, and the recent interest in G2G soil moisture outputs makes this a timely evaluation. The aims of this study are therefore to:

i. Understand how well G2G captures annual and seasonal soil moisture by evaluating it against a newly collated dataset of NP observations;
ii. Identify the areas (regions or landscape characteristics) where G2G is able to capture soil moisture patterns, and areas where improvements are needed;
iii. Explore how errors in modelled soil moisture compare to possible uncertainties in the observations.

This will give a better understanding of the skill of G2G soil moisture simulations, helping to identify which applications the G2G soil moisture estimates are suitable for, as well as identifying possible avenues for model improvement.

2. Methods

2.1. Observed soil moisture

2.1.1. The UK Soil Moisture Databank

Observed soil moisture measurements were extracted from the UK Soil Moisture Databank, hereafter UKSMD (Bell et al., 2022). The UKSMD collates in situ neutron probe measurements of soil moisture for over 100 sites across GB (see Fig. 1), collected between 1966 and 2003. The neutron probe technique uses the emission and detection of neutrons to provide a measure of the water content of the surrounding soil (Hollinger and Isard, 1994). Access tubes are fitted vertically into the soil, and neutron probes are lowered directly into these tubes to take measurements at various depths (Bell, 1987). The neutron probe readings are assumed to measure a sphere of soil around the probe, with a typical radius of 20 – 30 cm (Bell et al., 2022). The output from neutron probes can be directly related to soil moisture content, and it is therefore considered to be a relatively accurate method compared to other soil moisture measurement techniques such as Capacitance and Frequency Domain Reflectometry, Gamma Ray Attenuation and the Pressure Plate method (Bell, 1987; Dobriyal et al., 2012).

A key advantage of the UKSMD is the availability of soil moisture measurements throughout the soil column rather than just at the surface. The UKSMD included two forms of soil moisture data for most sites; 1) soil moisture content measured at specific depths, and 2) a depth-integrated profile moisture content (PMC) which averages soil moisture content throughout the soil profile to give the total water content down to a specific depth. Here, we used the PMC data (cm/m) as it is most comparable to the G2G soil moisture store. The use of cm/m units can be thought of as the equivalent depth of water per unit depth of soil. G2G simulates total soil moisture within the soil column and therefore does not explicitly take account of different depth profiles; this is why it was imperative to evaluate the model against depth-averaged rather than surface soil moisture observations.

In the UKSMD, the soil depths to which PMC values are provided varied depending on the original study for which the data were collected. Generally, neutron probe readings in the upper 20 cm of the soil profile are not accurate, and so readings at 20 cm or the next depth down were usually assumed to apply to the whole of the zone above. For many sites PMC was originally only provided from the surface to the maximum depth of the soil measurements, but for others, it was provided from the surface to specific depths of soil. For sites where original PMC values were missing, these were calculated for the UKSMD down to the maximum measurement depth (Bell

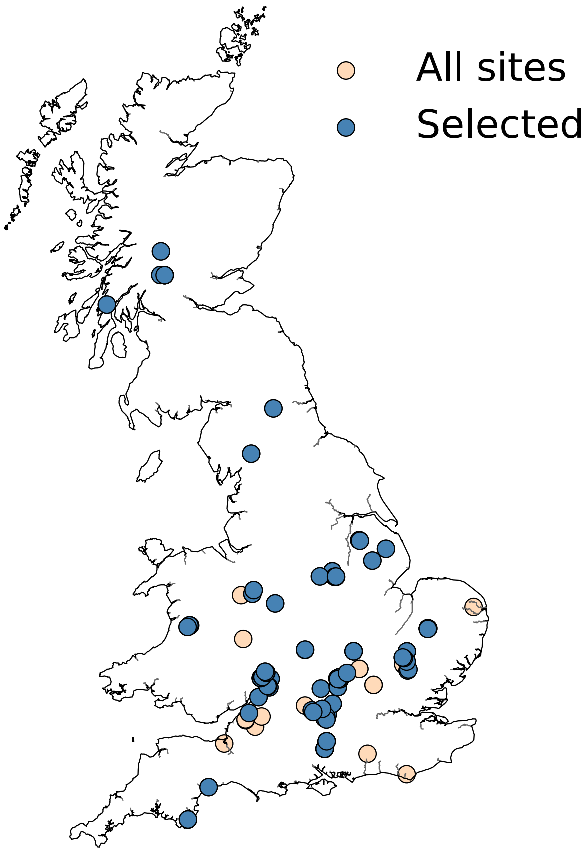

Fig. 1. Locations of UK Soil Moisture Databank sites where data was available and where data passed quality checks to be included in this study (blue).

et al., 2022). For the comparison with G2G depth-averaged soil-moisture undertaken here, we used the original PMC values from UKSMD where available and selected the depth closest to that used in the G2G. However, this did mean that the PMC depth varied between sites (the shallowest tubes measured down to 40 cm, the deepest tube down to 840 cm), due to differences in the measured depths.

2.1.2. Site selection

The measurements in the UKSMD were not completed as part of an overarching study, but rather the result of information from many independent studies collated into a common format (Bell et al., 2022). The data at different sites therefore varied in many aspects including 1) the time-period covered, 2) the frequency of measurements, 3) the number of tubes at a site, and 4) the quality of recorded meta-data. The mean record length was 4 years, but this varied from some sites measuring less than a year to one site measuring for almost 20 years. At some sites measurements were taken weekly without fail, at others measurements were taken monthly, but at many sites there was not a defined interval for the measurements or there were gaps in the time-series. While a few sites contained observations from a single tube, most (over 100) sites contained observations from three or more tubes, and one site in Scotland (Crinan) had 22 tubes.

Given the above limitations, a subset of the data were selected for use in this study. To be included sites had to have at least one tube which satisfied the following criteria: 1) at least 1 full year of measurements, 2) at least 12 measurements, 3) at least 1 measurement each meteorological season. These criteria aimed to retain as many sites as possible to evaluate the model nationally, while rejecting sites where the record was too short or incomplete to properly analyse the agreement between model output and observations throughout the year. The observed soil moisture time-series were then visually assessed for any suspect data. This resulted in the removal of data pre-1982 for the PLYNL_YF site, where investigation into a step-change in the observed data time-series identified errors in the recording of data. These criteria led to 112 sites being reduced to 85 (site locations are given in Fig. 1, details in Appendix C). The selected sites had a record length of 1–14 years (mean 3 years), and each site had between 15 and 805 soil moisture observations (mean of 96 observations per site). Unfortunately, the sites were not evenly distributed across Great Britain, with most sites located in England and Wales and only a few sites in northern England / Scotland.

2.1.3. Multi-tube sites and observational uncertainties

Where there were multiple tubes in the same site location a single tube was selected to include in the model performance analysis, to prevent overall results being skewed towards the unique conditions at a particular site. The final tube selected was the one with the closest match to the G2G model depth at the site location, and where multiple tubes had the same depth the one with the greatest number of measurements was chosen.

However, sites containing multiple tubes also provided a valuable opportunity to explore the uncertainty in soil moisture observations within a site, and thus to help understand the spatial variation in soil moisture within a 1 km model grid cell. The range in soil moisture observations across all tubes was calculated for each site. The mean range across all time-steps was then used as an indication of the spatial variation in soil moisture across the site and thus a 1 km model grid cell. There were 30 sites with measurements from 3 or more tubes that satisfied the site selection criteria outlined in Section 2.1.2. Of these, four sites contained tubes covering an area of over

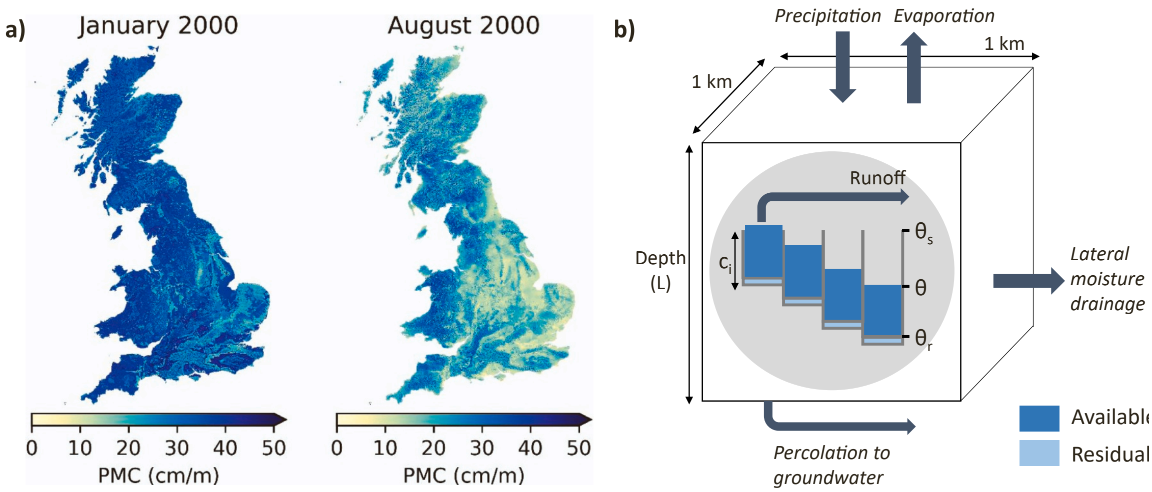

Fig. 2. Grid-to-Grid modelled soil moisture, including example maps of model output (a) and a simplified model structure diagram (b). Maps show the 1 km gridded profile moisture content averaged over January and August 2000. The simplified model diagram demonstrates how G2G simulates soil moisture. The multiple stores represent the PDM store formulation of Moore (2007) which assumes a distribution of storage capacities (c) across the modelling unit, here a grid cell. Simulated water content (θ) varies between saturation (θ_s) and residual (θ_r) water content, with runoff generated when soil moisture exceeds θ_s. Available soil water storage, (θ- θ_r)L, which contributes to runoff is represented in darker blue, residual water storage, (θ_r)L, which does not contribute to runoff is coloured in lighter blue.

1 km x 1 km (i.e. the easting/northing of the tubes differed by over 1000 m). As the focus was on possible uncertainties within a G2G grid cell, these very large sites were removed from the multi-tube analysis, with 26 sites remaining.

Sources of uncertainty in gridded moisture measurements include 1) the measurement uncertainties in the point-scale data, and 2) how representative point-scale data is of conditions across the wider area. Neutron probe measurements themselves can be relatively accurate, with reported accuracy of measured volumetric water content in the range +/- 0.001 – 0.002%, provided the probes have been calibrated correctly (IAEA, 2000; Lekshmi et al., 2014). However, the quality of the calibration (which defines the relationship between the number of neutron counts and volumetric soil moisture content) differs across the UKSMD, with some sites potentially having minimal calibration and others being calibrated with the assumption that soil type did not differ with depth (Bell et al., 2022). The scaling from a point source measurement provided by the neutron probe to the (1 km × 1 km) area average soil moisture simulated by G2G introduces further uncertainties due to the heterogeneity of soil moisture across the landscape (Crow et al., 2012). Exploring the range in observations across all tubes within a site provided a chance to understand these uncertainties. It is important to note that the scientific justification for measuring at multiple tubes differed between the sites, as measurements were obtained from independent studies that were subsequently collated into the UKSMD. Thus, some sites had multiple tubes covering different land-uses, soil types or soil management practices, whilst others had multiple tubes in more-similar environments. In both cases, the measurements were regarded as useful in helping to understand possible variations in observed soil moisture within a 1 km grid cell.

2.2. Simulated soil moisture

2.2.1. The Grid-to-Grid model

Grid-to-Grid (G2G) is a national-scale grid-based hydrological model, which simulates natural flows across GB (Bell et al., 2009). Alongside estimates of river flow, the model can output 1 km resolution, vertically-integrated soil moisture estimates, which are simulated at each model time-step as a precursor to calculating runoff and river flow (see Fig. 2a for example gridded soil moisture output and Fig. 2b for a simplified model structure diagram). G2G was originally developed for flood forecasting and hydrological climate impact analyses, but has also been used to investigate droughts, and changing river flows at the national scale (Bell et al., 2016, 2007b; Cole and Moore, 2009; Kay et al., 2018; Lane and Kay, 2021; Rudd et al., 2019, 2017). The model is also used operationally, for example contributing to the UK Hydrological Outlook monthly and seasonal river flow forecasts and also to the Environment Agency's national flood forecasting system (Bell et al., 2017; Price et al., 2012; Prudhomme et al., 2017).

G2G flow simulations have been comprehensively evaluated against observed river flows; these evaluations have not highlighted any regions of Great Britain where the model is consistently better/worse (Bell et al., 2009, 2007a; Rudd et al., 2017). However, Bell et al. (2009) found that river flow simulations were generally less accurate for catchments with artificial influences on the flow regime (e.g. abstractions / discharges: Rameshwaran et al., 2021), and for areas of complex sub-surface hydrology. G2G soil moisture simulations have been evaluated against MORECS (model-based) soil moisture (Kay et al., 2022a). However, no previous work has evaluated the modelled soil moisture against soil moisture observations.

2.2.2. Grid-to-Grid simulation of soil moisture

G2G-estimated soil moisture, θ, varies between the saturation (θ_s) and residual (θ_r) water content for the soil column, which is assumed to have a depth L (see Fig. 2). The whole soil column is treated as a single depth-integrated store, with no explicit modelling of different depth profiles. The actual water storage (S), maximum 'available' water storage ($S_{\max}$), and residual water storage ($S_r^{'}$) are given by

$$S = (\theta - \theta_r)L \tag{1}$$

$$S_{\max} = (\theta_s - \theta_r)L \tag{2}$$

$$S_r^{'} = \theta_r L \tag{3}$$

Soil water storage (S) increases when it rains, and is lost through evaporation, surface runoff and drainage. The residual water storage held under tension forces is not available for drainage but can contribute to evaporation. Evaporation losses are related to soil moisture through a simple function,

$$\frac{E_a}{E} = 1 - \left\{\frac{S_{\max} - S}{S_{\max} + S_r^{'}}\right\}^{2.5} \tag{4}$$

where (E_a/E) is the ratio of actual to potential evaporation, $(S_{\max} - S)$ is the soil moisture deficit and $(S_{\max} + S_r^{'})$ is the maximum total water stored.

To take account of spatial variability in soil-moisture across a 1 km grid-square, the probability-distributed soil moisture (PDM) store formulation of Moore, (2007) is invoked within each grid-square. Using the PDM, soil water storage in a grid square can be represented by a distribution of storage capacities to take account of how water absorption capacity can vary with soil, geology, land-cover and topography. This approach means that a total value of soil moisture (and surface runoff) is associated with each grid-square, but the grid-square is able to generate saturation-excess surface runoff even if it is not fully saturated, leading to more-realistic river flow estimates. The G2G formulation also allows for lateral moisture drainage (as shown in Fig. 2b), and thus each soil-column can gain or lose moisture to/from downstream/upstream grid-cells. Further details about G2G and how soil-moisture is estimated are provided by Bell et al. (2009).

The G2G parameters were previously estimated across Great Britain based on soil properties (Bell et al., 2009). Subsequent applications of G2G have used these national values with no additional calibration. For a fair assessment of model performance, this standard parameterisation was also applied here. For the soil moisture parameters, derived soils data from the Hydrology of Soil Types (HOST; Boorman et al., 1995) were linked with typical estimates of soil depth and hydraulic parameters. Specifically, soil parameters θ_s, θ_r, L, saturated hydraulic conductivity (k_s) and maximum total water storage (S_{max}) associated with each HOST class were estimated from soil and land cover datasets (Bell et al., 2009). Calibrated values of the PDM 'shape' parameter (b), which controls the degree of variability in storage capacity over the grid square, were found to have an inverse relationship to S_{max}. The b parameter was therefore estimated based on its relationship to S_{max}, except for areas of permeable geology with very deep stores (L > 1 m), where setting b to 0 was found to improve model performance. Importantly, this calibration process focused on model simulation of river flows and did not specifically calibrate for soil moisture.

2.2.3. Input data

The model requires gridded inputs of observed precipitation and potential evapotranspiration (PET). The UKCEH Gridded Estimates of Areal Rainfall (CEH-GEAR) product was used to provide 1 km gridded daily precipitation (Tanguy et al., 2019). This product uses rainfall estimates derived from the Met Office national database of observed precipitation, converted to a 1 km grid using the natural neighbour interpolation and a normalisation step based on average annual rainfall (Keller et al., 2015; Tanguy et al., 2019). The Met Office Rainfall and Evaporation Calculation System (MORECS) PE from short grass (i.e. assuming short grass cover everywhere) was used to provide monthly PET (Hough and Jones, 1997). This was converted from a 40 km grid to a 1 km grid, by simply assigning each 1 km grid cell the value of the 40 km grid cell within which it was contained. This PE product was chosen for a number of reasons; 1) It extends back through the 1960 s compared to HadUK-Grid PE which starts in 1969 (Brown et al., 2022), and 2) it is the product used in the initial G2G parameterisation and operationally used within the UK Hydrological Outlooks (Bell et al., 2017, 2009). The low spatial and temporal resolution of MORECS PE was not found to have a substantial impact on the modelled soil moisture compared to simulations using 1 km daily HadUK-Grid PE (see Appendix E). For this study, model simulations were carried out over the period 1964–2018, run at a 1 km resolution and 15-minute time-step. The first two years (Jan 1964 - Dec 1965) were used as a model spin-up period. Daily mean soil moisture time-series (G2G values) were saved for each of the grid cells corresponding to soil moisture observation sites.

2.3. Evaluation of model performance

2.3.1. Performance metrics

A range of performance metrics were calculated to assess the similarity between observed and simulated soil moisture time-series. For each site, metrics were calculated on days when both model simulations and observations were available, using only the single selected tube for observations. All metrics were calculated both annually and seasonally to evaluate whether model skill varied by season as soils became wetter and drier.

First, the bias was calculated to evaluate the agreement between the mean observed and simulated soil moisture values. The following equation was used;

$$bias = \overline{PMC_{sim}} - \overline{PMC_{obs}} \tag{5}$$

where $\overline{PMC_{sim}}$ is the mean of the simulated profile moisture content, PMC, and $\overline{PMC_{obs}}$ is the mean of the observed PMC.

Second, the error in the standard deviation was calculated to evaluate whether the model could correctly capture the variation in soil moisture throughout the whole time-series. This was calculated using

$$error\ in\ std = \sigma_{sim} - \sigma_{obs} \tag{6}$$

where σ_{sim} is the standard deviation of the simulated PMC, and σ_{obs} is the standard deviation of the observed PMC.

Finally the Pearson correlation coefficient was calculated to assess the overall agreement between the simulated and observed time-series.

2.3.2. Capturing wet / dry periods

Many users of the G2G soil moisture are interested in relative soil moisture values, focusing on when the soil is drier or wetter than normal as opposed to absolute values of soil moisture (Bell et al., 2017; UKCEH, 2022a). To evaluate relative soil moisture, each PMC data point was converted into a percentile of all the data points for that site (treating observed and simulated data points separately, and only using simulated data on days when observations were available). This allowed comparison of when PMC values were particularly high (above the 80th percentile PMC value) and low (below the 20th percentile PMC value).

To summarise this, the hit rate (HR), false alarm rate (FAR) and critical success index (CSI) were used. The hit rate evaluates the proportion of time that soils are correctly simulated as wet (i.e. above the 80th percentile of soil moisture values), and is calculated using

$$HR = (W_m \cap W_o)/(W_o) \times 100 \tag{7}$$

where $(W_m \cap W_o)$ is the number of wet days correctly simulated by the model and W_o is the number of wet days in the observed time series. The hit rate does not penalise over-prediction of wet days, which can instead be captured using the false alarm rate;

$$FAR = (W_m \cap \overline{W_o})/(W_o) \times 100 \tag{8}$$

where $(W_m \cap \overline{W_o})$ is the number of wet days simulated by the model when it was not actually wet (with $\overline{W_o}$ used to denote days that were not wet in the observed time series). The critical success index gives a more comprehensive measure of the agreement between simulations and observations, through

$$CSI = (W_m \cap W_o)/(W_m \cup W_o) \times 100 \tag{9}$$

where $(W_m \cup W_o)$ is the number of days that either observations or simulations are wet. The hit rate, false alarm rate and critical success index all return scores between 0 and 100, with higher scores indicating better performance for the hit rate and critical success index, and lower scores indicating better performance for the false alarm rate. The same calculations were repeated to calculate the hit rate, false alarm rate and critical success index for capturing dry days (i.e. below the 20th percentile of soil moisture values).

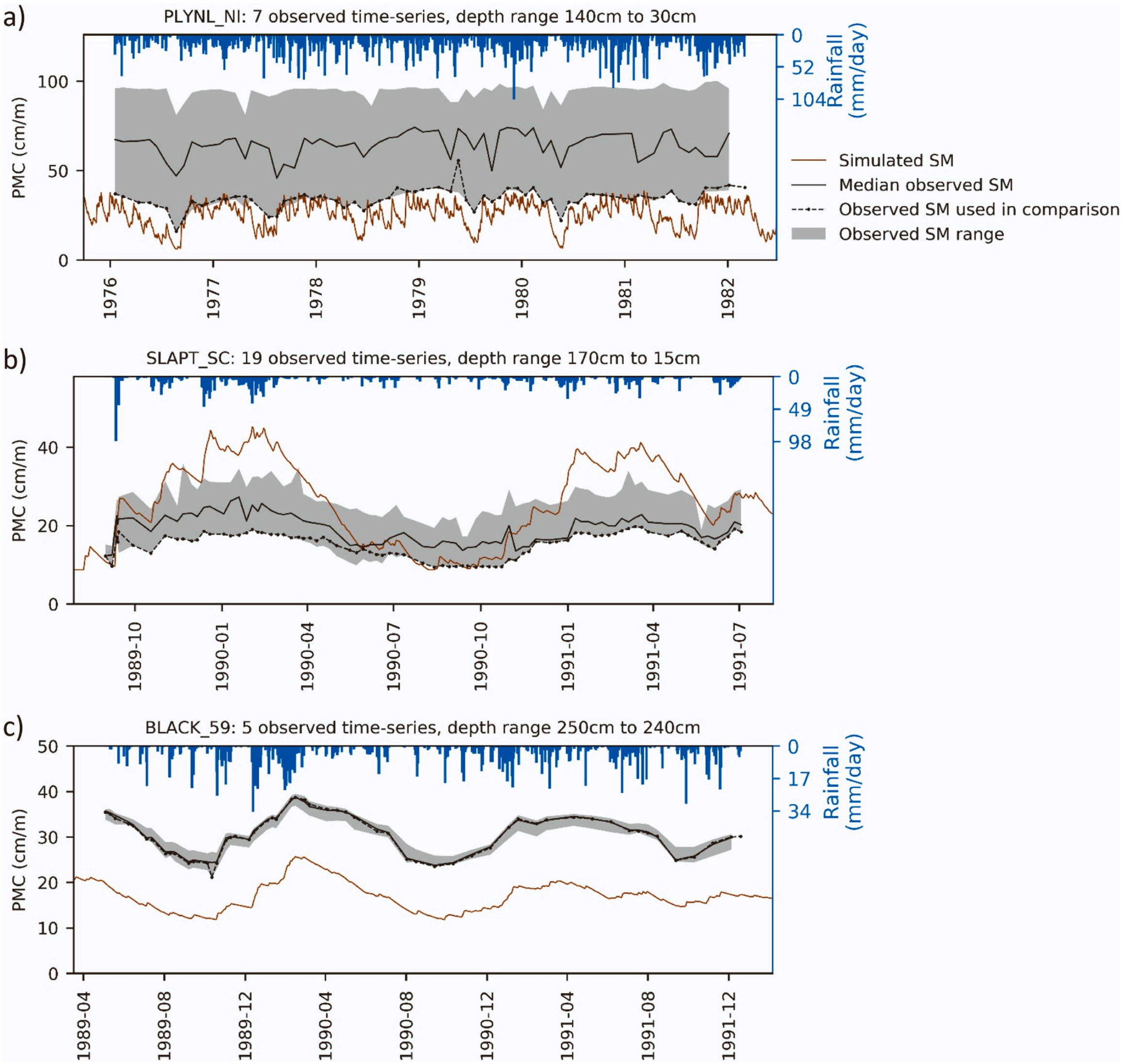

Fig. 3. Example profile moisture content (cm/m) and rainfall (mm/day) time-series from a selection of sites with multiple tubes. The G2G simulated soil moisture (brown line) is given alongside the observed soil moisture used in the model evaluation (black dashed line), as well as the median and range from all soil moisture observations at the site (black line and shading). The soil moisture time-series used in the model evaluation was selected to be the one with the most similar depth to the G2G soil moisture store, and the most measurements, so is not always close to the median soil moisture value. Plots a-c show the PLYNL_NI, SLAPT_SC and BLACK_59 sites respectively, which were chosen to demonstrate the variation in observed soil moisture ranges between sites. Bars on the top (right hand axis labels) show CEH-GEAR daily rainfall for the 1 km grid containing each site.

Calculating the *HR*, *FAR* and *CSI* metrics annually explores how well the model can capture the overall seasonal fluctuation in soil moisture values. However, a harder test is how well the model can capture events with relatively high/low soil moisture for each particular season. This analysis was therefore repeated seasonally, using only observed and simulated PMC values within each season. For this analysis, only the 40 sites with at least 12 observations in each season were included.

2.4. Landscape characteristics used in model evaluation

To further understand where and why the model skill in simulating soil moisture varied, the model performance was evaluated with respect to landscape characteristics. After evaluating soils and land-use, soil information from the Hydrology of soil types (HOST) dataset was found to be most informative (Boorman et al., 1995). HOST classifies soils across GB into 29 hydrologically distinct classes, based on datasets that described the soils, their distribution and the hydrological response of catchments (Boorman et al., 1995). Here, we use the properties of the dominant HOST class within a grid cell, including soil depth, soil composition and presence of groundwater. Maps showing dominant HOST soil depths and groundwater classes are given in Appendix A, alongside information on how HOST classes were grouped.

3. Results

3.1. Uncertainties in observed soil moisture within a site

The range in observed soil moisture was calculated for each time-step at each site containing multiple tubes within a 1 km x 1 km area. The mean range in soil moisture varied substantially between the sites, from 1.7 cm/m to 61 cm/m. The fact that there is this range in values highlights that while the model produces a single soil moisture value for a 1 km x 1 km grid, the soil moisture observations at individual locations within that grid could in reality be very different. Time-series of observed and modelled soil moisture are presented in Fig. 3 for a selection of multi-tube sites. These were chosen to help demonstrate the variation in observed ranges and

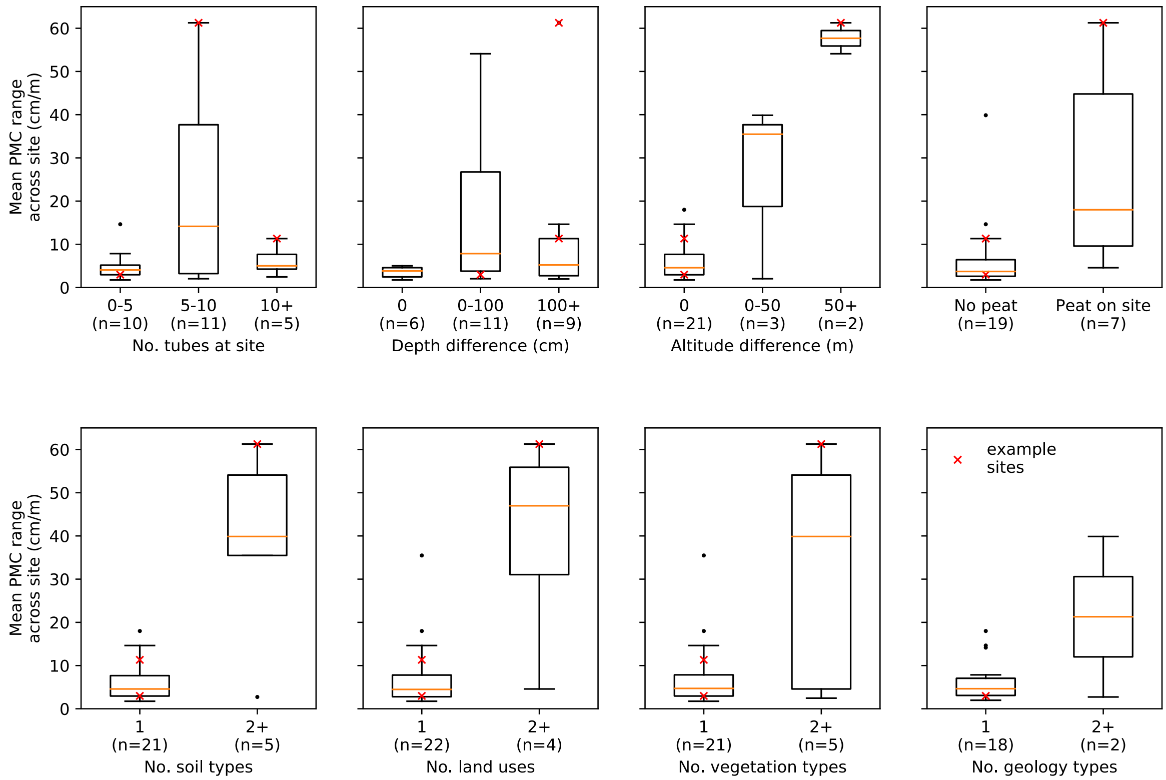

Fig. 4. Boxplots showing the PMC range across the 26 multi-tube sites, and various factors that could help explain variation in soil moisture within a site. Factors included; 1) the number of tubes within the multi-tube site, 2) the difference/range in depths profile moisture content was calculated over within a site, 3) the altitude difference/range between tubes within a site, 4) whether peat was recorded as a soil type at any tube within the site, 5) the number of different soil types recorded at the site, 6) the number of different land uses recorded across the site, 7) the number of different vegetation types recorded across the site, 8) the number of different geology types recorded (note – geology was only recorded for 20 sites). The number of sites falling within each category is given in brackets below each boxplot. Results for the example sites in Fig. 3 are given as red crosses to show how they relate to other sites.

model performance.

The PLYNL_NI site (Fig. 3a), had the largest range in observed soil moisture values across tubes of all the multi-tube sites (joint with the CRINA_CR site, which is not shown). This demonstrates how large the uncertainties in observed soil moisture measurements within a site, and subsequently a model grid cell, could be. The mean range between the seven tubes at the PLYNL_NI site was 61 cm/m. For context, the median observed soil moisture was 66 cm/m. The tubes at this site were in locations with a large spatial variation in altitude (406 m to 525 m), land-use (three tubes on heathland, three tubes on grassland, one unrecorded), and soil type (three tubes in peat, two tubes in podzol, one tube in organic soil on scree and one unrecorded). The depth over which soil moisture was measured also varied between tubes, and for some tubes PMC was given for multiple depths, resulting in PMC records covering depths of 40 – 140 cm across the site. The CRINA_CR site had similar spatial variation, with 22 tubes covering different land-uses (heathland/woodland), soil types (peat/brown earth), depths (55 – 205 cm) and altitudes (168 – 241 m), but had tubes spread over a larger area (2×3 km).

Part of the reason the PLYNL_NI site had such a large range in observed soil moisture is that it included some tubes with exceptionally high PMC values, of over 95 cm/m. The tubes recording these high PMC values were both on peat soils. Peat can be expected to have high PMC values of over 70 cm/m during the winter (UKCEH, 2023b), but the exceptionally high values could also indicate errors in the observed soil moisture data. Possible explanations for these errors could include 1) issues with the calibration equation used to convert neutron counts into volumetric water content and subsequently PMC, 2) free water around the NP access tube affecting readings.

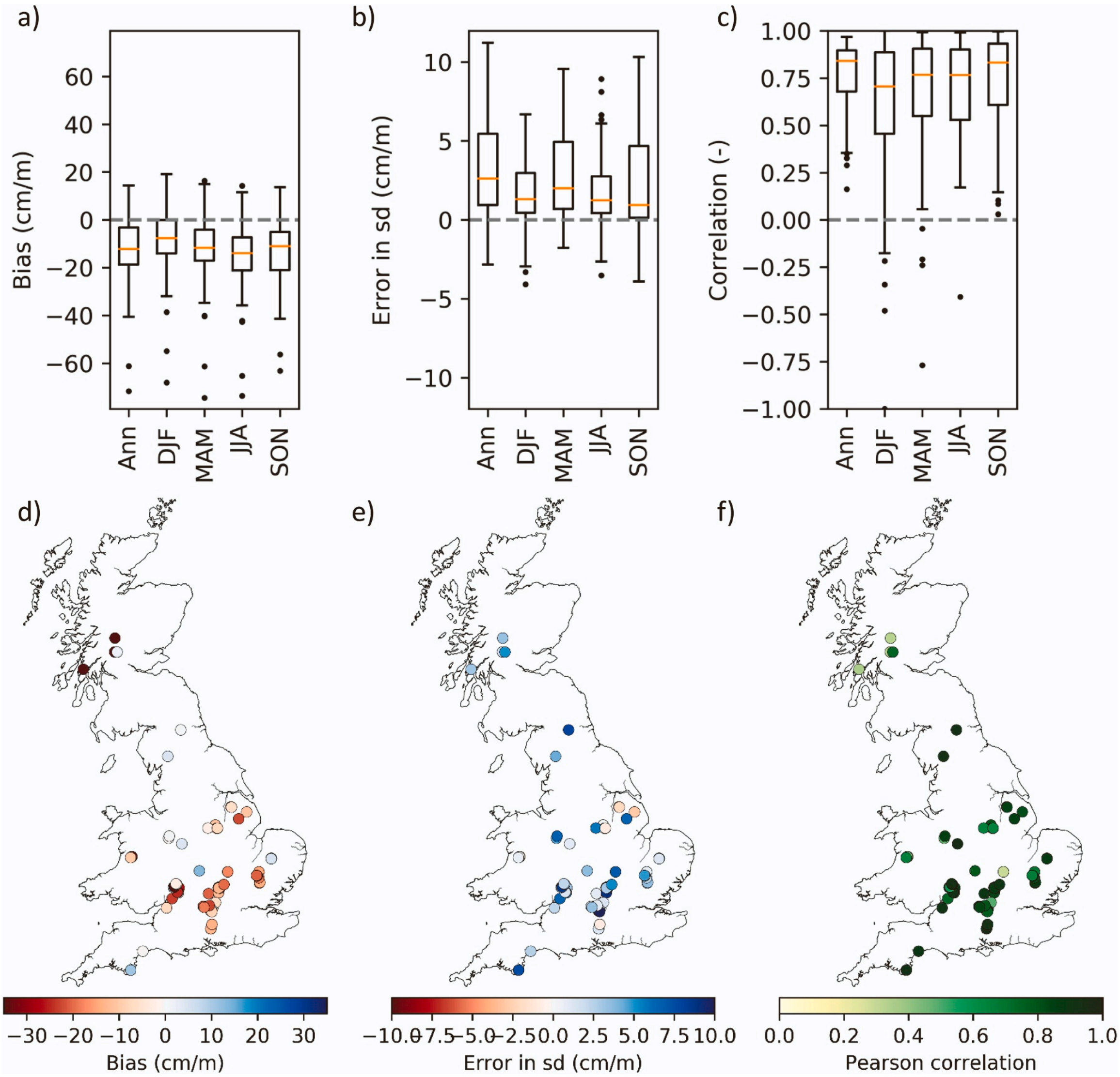

Fig. 5. Summary of model performance relative to observations across all sites, given as boxplots (a-c) and maps (d-f). Metrics shown are: Bias in mean simulated soil moisture, Error in the standard deviation of simulated soil moisture, and Pearson correlation coefficient, all calculated annually as well as for winter (DJF), spring (MAM), summer (JJA) and autumn (SON).

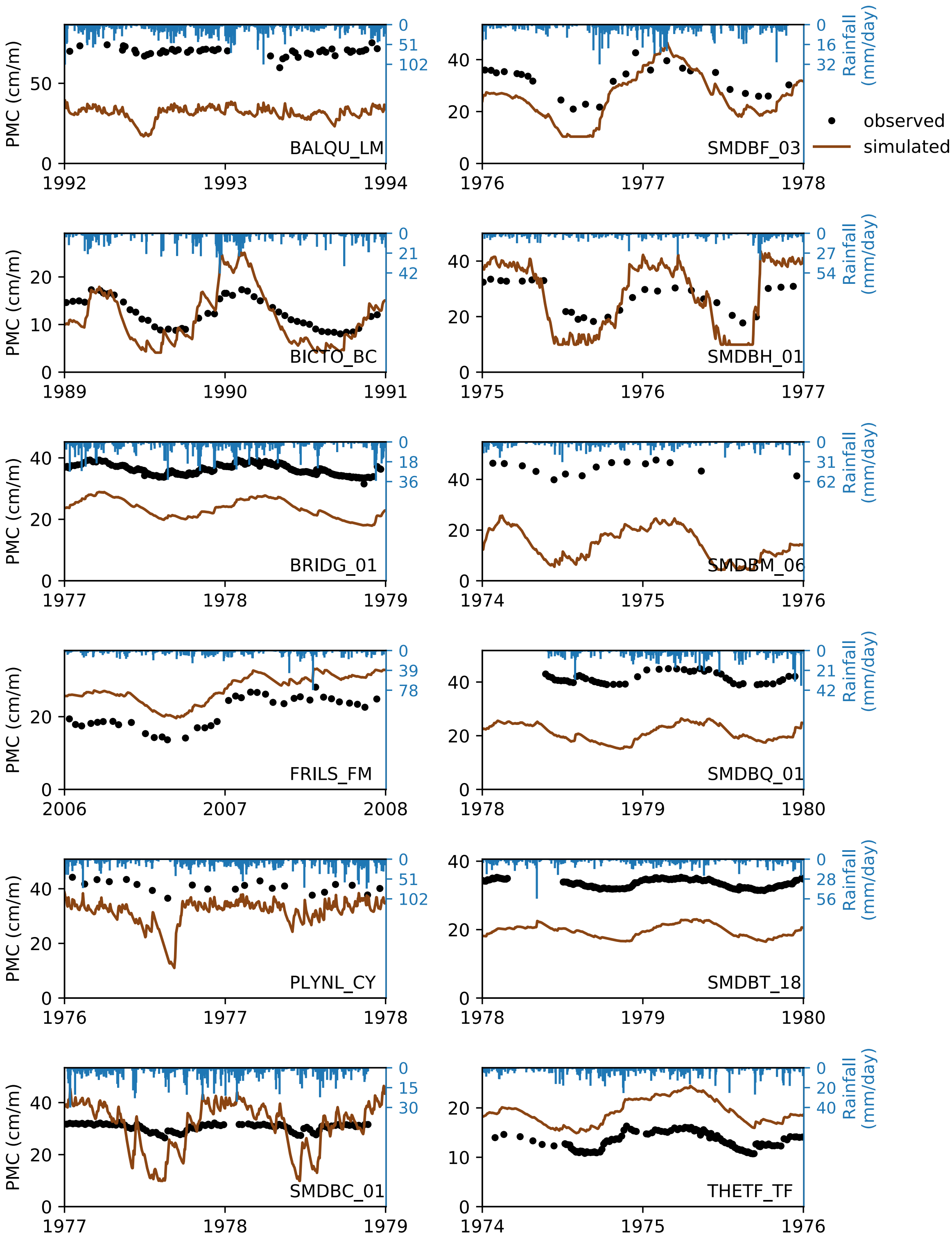

Fig. 6. Time series of profile moisture content from G2G simulations and UKSMD observations for 12 sites distributed across GB. Site IDs are given in the bottom right of each plot. A two-year period from January-December is shown for each site, but different years were selected due to data availability. Dots are given on the dates observed soil moisture measurements were available, demonstrating the differences in sampling frequency between sites. Daily simulation PMC data is shown, but only the days when observations were available were used in the model evaluation. Daily CEH-GEAR rainfall data for the 1 km grid containing each site is given on the right axis, to demonstrate the soil moisture response to rainfall.

The SLAPT_SC site (Fig. 3b), had a relatively large range (11 cm/m) in PMC values between tubes. This site had 19 unique tubes, all recorded as having the same grass/woodland land-use, stony brown earth and 101 m altitude. The key difference between the tubes at this site was the depth over which PMC was calculated, ranging from 65 – 170 cm. Soil moisture generally varies less with increasing depth; surface soil moisture is more likely to vary on daily to weekly time-scales with precipitation/ evaporation / vegetation changes,

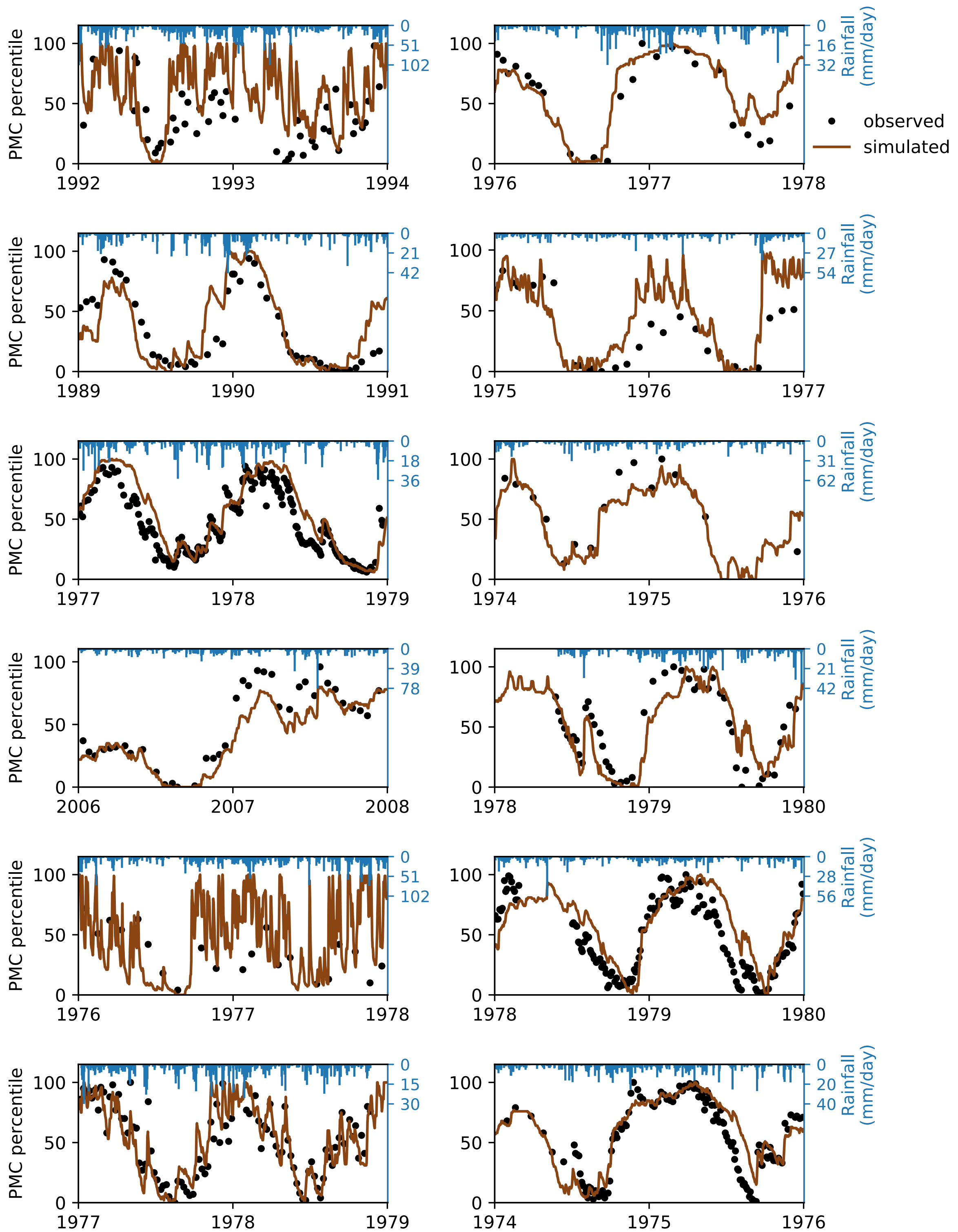

Fig. 7. As for Fig. 6, but showing time-series of the percentile of each PMC value. Sites are given in the same order as for Fig. 6.

while deeper soil moisture tends to be more stable with seasonal / annual variations. Over a typical year, PMC from shallower tubes would therefore be expected to have more variability than PMC from deep tubes.

The BLACK_59 site (Fig. 3c) had relatively small ranges in PMC values between tubes (2–3 cm/m). The five tubes at this site were recorded as having the same land use (ash woodland), soil type (shallow, organic-rich forest soil overlaying Cretaceous chalk), altitude (143 m) and measuring PMC to similar depths (240 – 250 cm).

The relationship between the range in observed PMC values across a site and various site properties are given in Fig. 4 for all multi-tube sites. Neither the number of tubes at a site nor the range of depths over which PMC was reported have a clear relationship with the range between observations at a site. The range in the observations is instead likely related to a combination of factors such as spatial variation in altitude, soil type, land use, vegetation and geology across the site (Fig. 4). The distance between tubes could also have had an impact, but tube locations were not given to a high enough precision to explore this. Sites containing some tubes with peat soils also tend to have large ranges in observed PMC. The three example sites from Fig. 3 have been plotted as red crosses, to show how they compare to the rest of the multi-tube sites.

3.2. *Evaluation of modelled soil moisture*

Fig. 5 summarises the performance of modelled soil moisture relative to observations across all sites. Results are given in the soil moisture units (cm/m). The G2G model tends to underestimate soil moisture relative to observations, with generally negative bias values throughout the year (Fig. 5a). Median bias values are −12 cm/m when evaluated annually. The underestimation tends to be largest in the summer (median bias −14 cm/m) and smallest over winter (median bias −8 cm/m), although there is much overlap between the seasons.

The model tends to over-estimate the variation in soil moisture values both annually and within each season (Fig. 5b), with simulated annual soil moisture having a larger standard deviation than observed soil moisture in 74 out of the 85 sites. The largest under-estimations of soil moisture tend to be in the summer when soils are usually driest, and the smallest under-estimations tend to be in winter when soils are usually wettest. Model over-estimations of the standard deviation could in part be due to observations under-estimating soil moisture variation, as much of the soil moisture variability is likely to be at the near surface, and NP readings could not be taken at depths shallower than 15–20 cm.

There is good correlation between observed and modelled soil moisture time-series at many sites (Fig. 5c), with annual Pearson correlation values exceeding 0.7 for 61 sites, and exceeding 0.9 for 20 sites. Correlation tended to be better in autumn and worse in winter.

The spatial distribution of model performance relative to observations is shown in Fig. 5d-f. There are no clear overall patterns of model performance. The largest model under-estimates of soil moisture are in western Scotland, whereas over-estimates of soil moisture appear to be mainly distributed in central and northern England. The few sites where the model under-estimates the variation in soil moisture are mostly clustered in the East Midlands. However, unfortunately the high spatial coverage of soil moisture sites across central and south-eastern England, and lack of sites covering large areas of Scotland, northern England and Wales, makes it difficult to draw any firm conclusions regarding spatial patterns of model performance.

Time-series of profile moisture content are given for 12 sites in Fig. 6. These 12 sites were selected as examples because they were distributed across GB and cover a range of model performance (site locations and performance summaries are given in Appendix B, and time series for all sites are provided in Appendix D). These time-series show how individual sites contribute to the overall performance statistics reported in Fig. 5; the tendency of the model to under-estimate soil moisture values and over-estimate the variation in soil moisture can be seen across these time-series. In some cases there are large negative biases all year round (e.g. BALQU_LM, SMDBM_06, SMDBT_18), in other cases we see positive winter biases alongside negative summer biases due to the overestimation of soil moisture annual variation (e.g. BICTO_BC, SMDBH_01), and a few sites show consistent positive biases (e.g. THETF_TF). It can also be seen that the model is able to capture the seasonal timing of soil moisture variation for many sites.

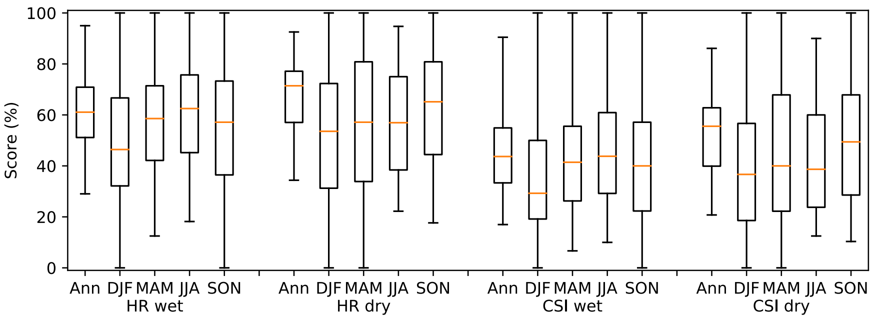

Fig. 8. Hit Rate (HR) and Critical Success Index (CSI), for capturing wet days (when the observed PMC is above the 80th percentile) and dry days (when the observed PMC is below the 20th percentile) calculated annually and seasonally. Boxplots show the range across the 40 sites that have at least 12 observations for each season (see Appendix E for annual results across all sites and values for the false alarm rate). Higher values indicate better model performance, with a score of 100 indicating perfect performance.

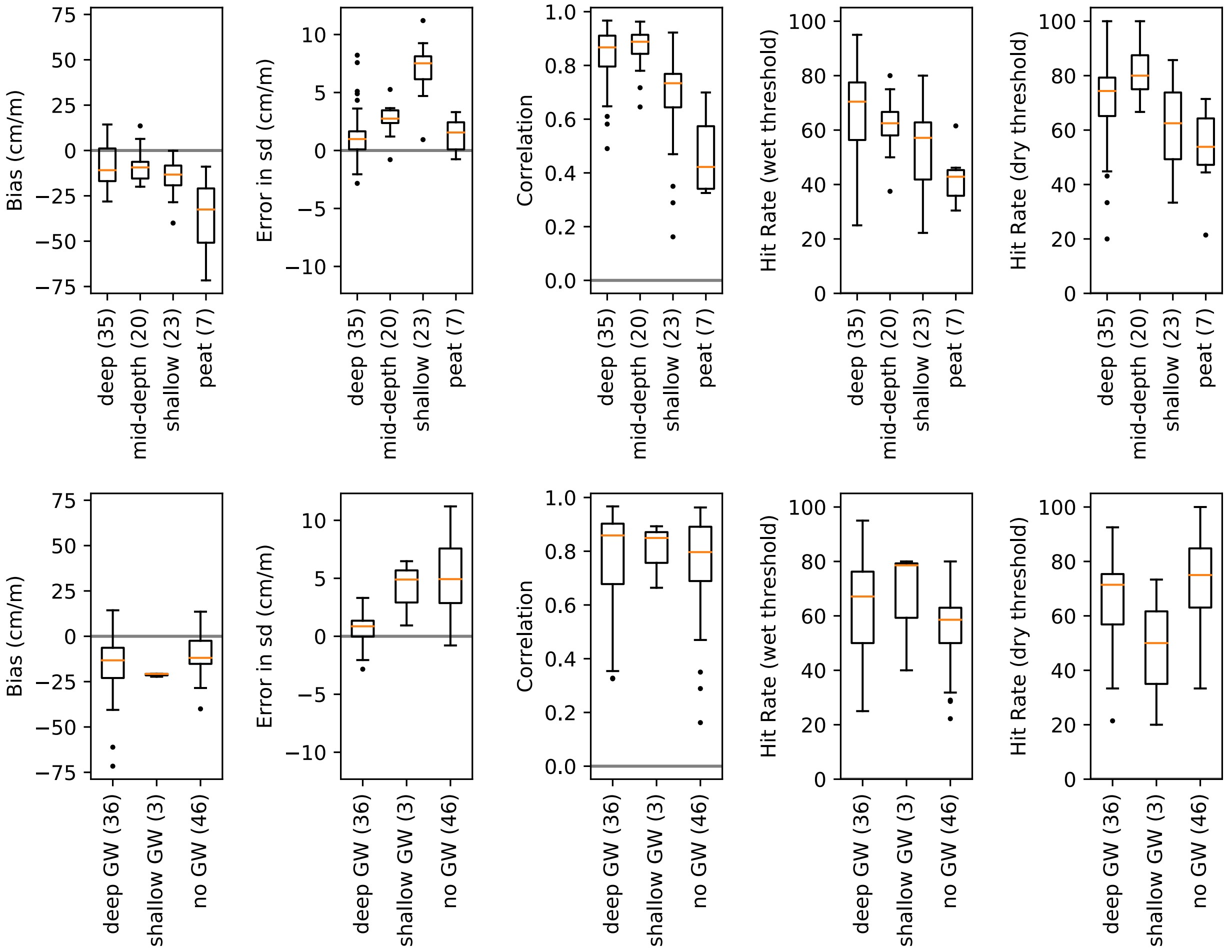

Fig. 9. Summary of model performance relative to observations when sites are separated by soil and groundwater depth (see Appendix A for explanation of categories). The top row separates sites by soil depth, with peat soils also evaluated separately to mineral soils. The bottom row separates by groundwater depth. The number of sites falling into each category is given in brackets on the x axes labels. The first column shows bias in annual mean simulated soil moisture, second column shows error in the annual standard deviation of simulated soil moisture, third column shows Pearson Correlation, fourth column shows the hit rate for capturing wet soil moisture (i.e. when observations exceed the 80th percentile for soil moisture, what percentage of the time do simulations also exceed the 80th percentile), and the fifth column shows the hit rate for capturing dry soil moisture (i.e. below the 20th percentile).

3.3. Evaluation of modelled relative wetness/dryness

Time-series of profile moisture content percentiles are shown in Fig. 7 for the 12 selected sites, with time-series for all sites given in Appendix D. These provide a direct comparison of the observed and simulated relative soil wetness, and allow for an easier comparison of timing. For many of the sites, the modelled and observed time-series show good agreement during periods when soils are relatively wet and relatively dry (e.g. BICTO_BC, BRIDG_01, SMDBC_01). For a couple of sites, this analysis highlights good agreement overall but small offsets in timing between the model estimates and observations when soils are transitioning from wet to dry (e.g. BRIDG_01, SMDBT_18, THETF_TF). There are also a couple of sites where the model is able to capture broad seasonal patterns of relative wetness, but the agreement between the modelled and observed soil moisture remains poor (BALQU_LM, PLYNL_CY). These sites both contain areas of peat soil.

Fig. 8 summarises how well the model can capture when the soil moisture observations are relatively wet/dry, showing the range across sites with at least 12 observations in each season (the range across all sites is given in Appendix E). The median result across all sites for how well the model can capture wet (dry) days is a hit rate of 62 (73), a false alarm rate of 38 (27) and a critical success index of 44 (58). In other words, when observed soil moisture is very wet (i.e. above the 80th percentile), ~60% of the time simulated soil moisture is also very wet, and when observed soil moisture is very dry, ~70% of the time simulated soil moisture is also very dry. The model is better at capturing dry days, with a generally higher hit rate and lower false alarm rate than for wet days.

Capturing whether soils are relatively wet/dry for a particular season presents a harder challenge for the model. Overall, the model is slightly better at capturing relatively wet days in summer and relatively dry days in autumn, with the model least able to capture relative wetness/dryness in winter.

3.4. Performance breakdown by landscape characteristics

Fig. 9 (top row) shows how model performance varies between G2G grid cells with different soil depths/types. Sites on deep, mid-depth and shallow mineral soils all had similar biases, with the model generally under-estimating soil moisture, although there was a slight tendency towards larger under-estimations for shallower soils. However, there was a clear distinction between model biases for these mineral soils and for peat soils. The median annual bias for mineral soils was −12 cm/m, while the median model bias for peat soils was −33 cm/m. It is worth noting that there were only seven sites with peat soils.

The error in the standard deviation of modelled soil moisture also varied between the sites with different soil depths/types. Generally, the sites with shallower soils had higher errors in their standard deviation (i.e. larger over-estimation of the time-series variance) compared to observations. Median errors in the standard deviation were 1.0 cm/m, 2.7 cm/m, and 7.5 cm/m for deep, mid-depth and shallow soils respectively. Standard deviation errors for peat soils were not notably different to those from the deep and mid-depth mineral soils, with a median value of 1.6 cm/m.

There was generally a better correlation between observed and simulated soil moisture at the sites with deep and mid-depth soils, than at the sites with shallow or peaty soils. Median correlation values were 0.9 for sites with deep and mid-depth soils, reducing to 0.7 for sites with shallow soils, and 0.4 for sites with peaty soils.

There were no major differences in model bias or correlation when comparing the sites with deep groundwater to sites with no groundwater (Fig. 9 bottom row). However, the presence of groundwater did appear to relate to the error in the standard deviation of modelled soil moisture. Sites with no or only shallow groundwater tended to over-estimate the standard deviation, with median over-estimates of 4.9 cm/m. Sites with deep groundwater stores were more balanced, with both over- and under-estimates of the standard deviation, and a lower median error of 0.9 cm/m.

4. Discussion

The G2G model was developed with the primary aim of simulating river flows, and has been widely used and evaluated for this purpose (Bell et al., 2009, 2007a; Kay et al., 2021a; Lane and Kay, 2021; Rudd et al., 2017). However, there is growing interest in the depth-integrated soil moisture estimates simulated by G2G, which have already been used to explore questions such as how soil moisture timing and soil moisture droughts may be altered by climate change (Kay et al., 2022a; Rudd et al., 2019). Here, for the first time, we have evaluated the G2G soil moisture simulations against in situ soil moisture observations, to see if the G2G soil moisture estimates are informative. It is important to emphasise that there are many reasons G2G might not produce good soil moisture estimates, including: 1) The model parameters have not been calibrated with respect to soil moisture simulation, but were instead estimated nationally based on soil properties (Bell et al., 2009); 2) a relatively simple model structure is applied that was developed primarily for river flow simulation; 3) the model is usually applied nationally at a relatively course 1 km resolution so could not be expected to capture local variation in soil moisture. Following this evaluation of the current version of G2G, future work can focus on improving G2G soil moisture simulation.

The evaluation showed an overall good correlation between modelled and observed profile moisture content across GB, with the model generally able to capture wet and dry periods. This is a promising result, especially given the various differences between the observed and simulated data (including the spatial scale, PMC depth, and difference between what the hydrological model conceptualises as soil moisture and what is measured). However, G2G was generally less successful at reproducing the actual values of observed profile moisture content. There was a tendency for the model to under-estimate soil moisture, especially during the summer, and over-estimate the variation in soil moisture throughout the year (though this could partly be attributed to NP observations not-providing soil moisture estimates in the highly variable top 15–20 cm of the soil-column). Model under-estimation of soil moisture compared to observations was also found in previous evaluations focusing on different models and different observational soil moisture datasets (Oogathoo et al., 2022; Peng et al., 2021; Xia et al., 2014).

The generally good correlation between modelled and observed soil moisture indicates that the modelled soil moisture can be useful for simulating the seasonal variation in soil moisture, even if the model biases mean it is not suitable for predicting actual soil moisture values. This was supported by the agreement between observed and simulated soil moisture percentiles, especially when soils are dry. This result most likely reflects the fact that in many hydrological models, including G2G, it is change in soil moisture storage that really influences downstream river flows, rather than soil moisture absolute values. Most hydrological models are developed to simulate flows and supported by readily-available observed flow data, so it is unsurprising that absolute soil moisture values are less well represented (and understood).

Current users of the G2G soil moisture tend to be interested in the relative state of soil moisture, rather than the values themselves. For example, the UK Hydrological Outlook produces maps of the G2G simulated subsurface water storage anomaly, calculated as the storage difference from the historical monthly mean, to identify areas which are particularly wet/dry (Bell et al., 2013; UKCEH, 2022a). These data are freely available online, via a web app developed by the ASSIST project (UKCEH, 2023c, 2022b). A recent study on climate change impacts on soil moisture focussed on the relative changes in occurrence of soil moisture extremes and wetting/-drying dates (Kay et al., 2022a, 2022b). Our results support these uses of the G2G soil moisture, as it has shown to be informative in simulating relative values.

There is a wide interest in large-scale soil moisture information, including for agricultural applications, flood forecasting, drought monitoring, landslide management and climate change adaptation studies (Bolten et al., 2010; Jalilvand et al., 2019; Nendel et al., 2014; Wanders et al., 2014; Wicki et al., 2020). Given the sparse nature of in situ soil moisture observations, and the limited depth of satellite observations (surface to 5 cm), modelled soil moisture can help to fill this need. For example, soil moisture information at greater depths is important for agriculture, where roots of winter wheat and oilseed rape, both widely grown UK crops, tend to reach 50 cm deep and can extend to 60 / 77 cm respectively (White et al., 2015). Farmers could use current relative soil moisture to support effective irrigation scheduling across large scales and long-term future relative soil moisture to inform climate change adaptation such as a switch to drought-resistant crops. Modelled soil moisture could also be used in conjunction with satellite information, to combine the best properties of both (Peng et al., 2021). While G2G has a very simple representation of soil moisture, for example when compared with the JULES land surface model (Best et al., 2011), our results indicate that G2G provides useful relative soil moisture information.

The model struggled to simulate soil moisture in peat soils, with generally larger biases and lower correlation between observed and simulated soil moisture in the grid cells that were predominantly peat. This could be due to the model being less able to represent processes in peatlands, or the large uncertainties in observations for areas with peat soils. Peng et al., (2021) also found that the JULES model had a lower correlation with COSMOS-UK soil moisture measurements for stations with organic soils. This was attributed both to limitations in the JULES model's representation of organic soil processes, and uncertainties in COSMOS measurements over organic soil. Peatlands can be difficult to model as the hydraulic properties depend on many factors including the pore structure, stage of decomposition, botanical composition and gas bubbles (Liu and Lennartz, 2019), none of which are represented in the G2G model. The water levels in peatland can also often be artificially managed, and no management is included in the G2G model. Furthermore, peat can expand and contract with changes in soil moisture (Price and Schlotzhauer, 1999). This expansion/contraction may mean that wet/dry periods are not as noticeable in the volumetric water content time-series. For example, Price and Schlotzhauer, (1999) observed no changes in volumetric water content of a peat soil during a wetting event because the peat expanded and the additional moisture was held in a larger overall volume. The original G2G parameterisation mainly focused on performance for areas with mineral soils, and therefore poorer representation of peatland processes is not surprising. Previous studies have found that a separate approach to simulate peat and mineral soils can lead to better results (Lane et al., 2021; Liu and Lennartz, 2019). Therefore, improving G2G representation of hydraulic properties in peatlands is a potential avenue for future research.

There are limitations to using in situ observed soil moisture data as an indicator of model performance. These include: 1) uncertainties in soil moisture measurements, 2) the difference in spatial scale between point-source observations and a relatively coarse modelled 1 km square, and 3) differences in depth between modelled soil moisture and observations. These all present challenges, and mean it is not a like-for-like comparison. Here, we have shown that the profile moisture content measured at multiple tubes within a 1 km square can differ by up to 61 cm/m, or up to 92% of the average PMC value. This is larger than the typical range for hydrologic data uncertainties, which McMillan et al., (2018) found to be around 10–40% (when considering point-scale data including rainfall, river levels and river flows). These large uncertainties and high spatial heterogeneity of soil moisture complicate model vs observation comparisons, as it is difficult to disentangle whether model results are poor or if the observations are not representative of processes at the spatial scale of the model grid-cells.

The variability of observed soil moisture within some of the 1 km model grid cells, particularly in areas with spatially varying landscape characteristics (e.g. soil type, altitude, land cover), highlighted the difficulty of modelling at a 1 km grid resolution. This model spatial resolution is useful for providing a national overview of the state of deeper sub-surface soil moisture, and soil moisture changes.

5. Conclusions

Grid-to-Grid soil moisture estimates could be a useful resource for a wide range of applications including for agricultural applications, flood forecasting, drought monitoring and landslide management. This work presents the first evaluation of Grid-to-Grid simulated soil moisture against a dataset of in situ neutron probe observations covering 85 sites across Great Britain. There was a good correlation between observed and simulated soil moisture for many sites (median correlation coefficient of 0.84), but the model tended to under-estimate soil moisture values throughout the year (median annual bias of −12 cm/m) and over-estimate the variation compared to observations (median standard deviation error of 2 cm/m). Using the relative state of modelled soil moisture (i.e. whether soils were wetter or drier than normal) was found to be more informative than using actual modelled soil moisture values. Model results should be treated with caution for shallow and peat soils, which generally had larger biases and a lower correlation with observations than deep or mid-depth mineral soils.

As well as improving understanding of G2G simulated soil moisture, this evaluation highlighted the difficulties of comparing point-source in situ observations with large-scale modelled soil moisture. Within a 1 km area, observations were found to differ by as much as 61 cm/m. These observational ranges were generally largest for sites with large variations in altitude or multiple soil, land use or vegetation types. The methods and results in this analysis will be of interest to a wide variety of users, for example 1) enabling users of G2G derived soil moisture data to better understand the model capabilities and limitations, 2) providing methods and a benchmark of performance for evaluations of soil moisture from other models, and 3) introducing the UK soil moisture databank which others could use in model evaluations.

CRediT authorship contribution statement

Alison L. Kay: Writing – review & editing, Supervision. **Rhian M. Chapman:** Writing – original draft, Conceptualization. **Victoria A. Bell:** Writing – review & editing, Supervision, Funding acquisition, Data curation, Conceptualization. **Rosanna A. Lane:** Writing – review & editing, Writing – original draft, Visualization, Methodology, Investigation, Formal analysis, Conceptualization.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data Availability

Data will be made available on request. The UK Soil Moisture Databank is openly available in the Environmental Information Data Centre at https://doi.org/10.5285/450bb14b-c711-47af-8792-f9bd88482cd4 (Bell et al. 2022). Monthly G2G soil moisture grids are available on the EIDC at https://doi.org/10.5285/c9a85f7c-45e2-4201-af82-4c833b3f2c5f (Kay et al., 2021b). The daily G2G soil moisture time-series used within this study are available from https://doi.org/10.5281/zenodo.7504041 (Lane and Bell, 2022).

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Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.ejrh.2024.101735.

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