



Estimation and evaluation of high-resolution soil moisture from merged model and Earth observation data in the Great Britain

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ABSTRACT

Soil moisture is an important component of the Earth system and plays a key role in land-atmosphere interactions. Remote sensing of soil moisture is of great scientific interest and the scientific community has made significant progress in soil moisture estimation using Earth observations. Currently, several satellite-based coarse spatial resolution soil moisture datasets have been produced and widely used for various applications in climate science, hydrology, ecosystem research and agriculture. Owing to the strong demand for soil moisture data with high spatial resolution for regional applications, much effort has recently been devoted to the generation of high spatial resolution soil moisture data from either high-resolution satellite observations or by downscaling existing coarse-resolution satellite-based soil moisture datasets. In addition, land surface models provide an alternative way to obtain consistent high-resolution soil moisture information when forced with high-resolution inputs. The aim of this study is to create and evaluate high-resolution soil moisture products derived from multiple sources including satellite observations and land surface model simulations. The JULES-CHESS simulated soil moisture and satellite-based soil moisture datasets including SMAP L3E, SMAP L4, SMOS L4, Sentinel 1, ASCAT, and Sentinel 1/SMAP combined products were first validated against observed soil moisture from COSMOS-UK, a network of in-situ cosmic-ray based sensors. Second, an approach based on triple collocation was applied to compare these satellite products in the absence of a known reference dataset. Third, a combined soil moisture product was generated to integrate the better-performing soil moisture estimates based on triple collocation error estimation and a least-squares merging scheme. From further evaluation, it is found that the merged soil moisture integrates the characteristics of model simulation and satellite observations and particularly improves the limited temporal variability of the JULES-CHESS simulation. Therefore, we conclude that the triple collocation merging scheme is a simple and reliable way to combine satellite-based soil moisture products with outputs from the JULES-CHESS simulation for estimating model-data fused high-resolution soil moisture for the British mainland.

1. Introduction

Soil moisture plays an important role in the Earth system, controlling surface runoff, infiltration, and the partition of surface energy fluxes (e.g., Koster et al., 2004; Miralles et al., 2014; Seneviratne et al., 2010; Taylor et al., 2012). Therefore, spatially and temporally accurate soil moisture information is significant for a wide range of applications such as Numerical Weather Prediction (de Rosnay et al., 2014; de Rosnay

et al., 2013), climate modeling (Seneviratne et al., 2013; Van den Hurk et al., 2016), flood forecasting (Crow et al., 2017; Massari et al., 2018), and drought monitoring (Martínez-Fernández et al., 2016; Nicolai-Shaw et al., 2017; Peng et al., 2020b).

Satellite remote sensing – particularly microwave remote sensing – has been widely applied to estimate surface soil moisture from regional to global scales (e.g., Babaeian et al., 2019; Brocca et al., 2017; Dorigo et al., 2017; Peng et al., 2021; Wagner et al., 2007). Currently, there are

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several global soil moisture products provided by different satellite-borne sensors such as Soil Moisture and Ocean Salinity (SMOS) (Kerr et al., 2010), Soil Moisture Active Passive (SMAP) (Entekhabi et al., 2010), Advanced Microwave Scanning Radiometer2 (AMSR2) (Kim et al., 2015) on board the Global Change Observation Mission-Water (GCOM-W), and Advanced Scatterometer (ASCAT) (Bartalis et al., 2007) on board the Metop satellites (Metop-A, Metop-B, and Metop-C). These products usually have moderate temporal resolution (1–2 days) and coarse spatial resolution from 25 to 50 km.

However, soil moisture products with high spatial resolution (< 10 km) are highly desirable for many regional applications (Leng et al., 2014; Merlin et al., 2008; Peng et al., 2016; Sabaghy et al., 2020; Su et al., 2020). Taking advantage of high-resolution Copernicus Sentinel 1 Synthetic Aperture Radar (SAR) observations, a 1 km soil moisture product over Europe has been produced and distributed by the Copernicus Global Land service (Bauer-Marschallinger et al., 2018). In addition, various downscaling approaches have been developed to improve the spatial resolution of global soil moisture products (Peng et al., 2017). For example, National Aeronautics and Space Administration (NASA) has recently released the fused SMAP/Sentinel 1 active-passive high-resolution soil moisture product at 3 km (Das et al., 2019). High-resolution SMOS soil moisture at 1 km has also been produced via the fusion of SMOS microwave with Moderate Resolution Imaging Spectroradiometer (MODIS) optical observations (Portal et al., 2020).

An alternative way to obtain high-resolution soil moisture estimates is through model simulation. With high-resolution meteorological forcing data as inputs, the land surface model simulated soil moisture has the advantages of self-consistency and completeness. Models are also able to simulate soil moisture to deeper layers in the root zone (Reichle et al., 2017a). Various simulation studies have computed soil moisture at different spatial scales with a wide range of models (e.g., Gebler et al., 2017; Samaniego et al., 2018). The accuracy of simulated soil moisture is closely related to the accuracy of model parameterization and the quality of meteorological forcing data (Pinnington et al., 2018; Vereecken et al., 2016). Recently, a long-term high-resolution soil moisture dataset (CHES-land) was generated with the Joint UK Land Environment Simulator (JULES) based on 1 km meteorological forcing data for the UK (Martinez-de la Torre et al., 2018; Robinson et al., 2017; Robinson et al., 2020).

While high-resolution soil moisture datasets offer potential for various regional applications, comprehensive assessment of these products is essential for their further improvement and to provide guidance on their suitability for potential applications (Gruber et al., 2020; Loew et al., 2017; Zeng et al., 2019; Zeng et al., 2015b). The validation of satellite-based products is typically conducted via direct comparison with ground-based soil moisture measurements at point-scale (e.g., Al-Yaari et al., 2019; Albergel et al., 2012; Colliander et al., 2017; Ma et al., 2019; Zeng et al., 2015a). Although the ongoing establishment of dense soil moisture networks across the globe can relieve the scale mismatch between ground-based measurements and satellite estimates, robust evaluation of satellite products in areas with sparse or no soil moisture networks remains challenging. To address this challenge, novel measurement techniques such as the Cosmic-ray Soil Moisture Observing System (COSMOS) have been investigated to measure soil moisture with a footprint around 700 m in diameter (Bogena et al., 2015; Evans et al., 2016; Zreda et al., 2012). Compared with traditional soil moisture measurements at point scale, the COSMOS soil moisture measured with a relatively large footprint is more suitable for validating satellite-derived soil moisture as well as modeled soil moisture (Montzka et al., 2017). Several studies have successfully evaluated satellite-based coarse soil moisture products using COSMOS soil moisture measurements over different areas such as Australia, Kenya, Germany, India, and the United States (Duygu and Akyurek, 2019; Kędzior and Zawadzki, 2016; Kim et al., 2015; Montzka et al., 2017; Mwangi et al., 2020; Upadhyaya et al., 2021). To facilitate water resources and environment related applications, the UK Centre for Ecology &

Hydrology has established and maintained a long-term and spatially-dense COSMOS network for the United Kingdom (COSMOS-UK) since 2011 (Evans et al., 2016). In the present study, the soil moisture measurements from COSMOS-UK are used as the reference dataset for the validation of the above-mentioned high-resolution soil moisture products with grid size at kilometer scale. The good practice guidelines for soil moisture validation provided by Gruber et al. (2020) are applied in this analysis. Evans et al. (2016) compared COSMOS-UK observations with a single satellite product (ASCAT) for two sites, as a demonstration of the potential of the network for evaluation of remotely sensed soil moisture. However, to our knowledge, this study is the first study that attempts to comprehensively evaluate existing high-resolution satellite soil moisture estimates and JULES simulation across the UK using COSMOS-UK measurements.

In addition to direct comparison with ground-based measurements, the triple collocation (TC) method has been explored to estimate error variances of geophysical variables (Gruber et al., 2016; Roebeling et al., 2012; Stoffelen, 1998). It has the advantage that there is no requirement for a reference dataset and the technique has therefore become an important method for evaluating satellite-based soil moisture products (e.g., Al-Yaari et al., 2014; Chen et al., 2018; Polcher et al., 2016; Su et al., 2014). In the present study, we also adopt the TC method to provide an independent assessment of high-resolution soil moisture products without specifying a reference dataset. It is expected that all of these products have individual error characteristics (Jackson et al., 2010; Loew et al., 2017). Several studies have demonstrated that merging different sources of products can lead to a better hybrid estimate (Gruber et al., 2017; Yilmaz et al., 2012; Zeng et al., 2016; Zhuang et al., 2020). For example, the European Space Agency's Climate Change Initiative for Soil Moisture (ESA CCI SM) team has chosen the TC-based method as the principal merging scheme for the generation of long-term harmonized soil moisture dataset with spatial resolution of 25 km based on multiple coarse-resolution satellite-based soil moisture products (Gruber et al., 2019b). Many studies have explored the improvement of model simulations through the assimilation of satellite products (e.g., Gruber et al., 2019a; Reichle et al., 2008), which is a more rigorous method than the TC-based merging approach (Crow and Van den Berg, 2010). However, the TC-based method has the advantage of being simple and transparent and is based on objective estimates of the relative error of various soil moisture products. To investigate and generate the best high-resolution soil moisture estimate for the UK in this study, the satellite-based and model-simulated soil moisture products are merged together based on error characteristics calculated using the TC method. The paper is organized as follows. Details of the satellite-derived products, JULES model simulated soil moisture and COSMOS measurements are described in section 2. The evaluation strategy and TC-based merging scheme are presented in section 3. The results are presented and discussed in section 4. Finally, the conclusions are given in section 5.

2. Data

2.1. Satellite-based soil moisture products

The satellite-based soil moisture products used in this study are listed in Table 1. More details of each product are introduced in subsections below. It is noted that these products represent soil moisture at the top surface (0–5 cm).

2.1.1. Sentinel 1

The Sentinel 1 satellites, operated by ESA, were launched in 2014 and 2016 to provide C-band (5.405 GHz) Synthetic Aperture Radar data with a typical spatial resolution of 20 m and a temporal resolution of 12 days at global scale (Torres et al., 2012). The frequent Sentinel 1 SAR data opens a new era for global high-resolution soil moisture estimation (Paloscia et al., 2013). Various methods with a range of complexity have

Table 1

Overview of the high-resolution satellite-based soil moisture products used in this study.

Soil moisture product	Temporal resolution	Time period	Coverage	Grid size	Original band frequency	Data Provider
Sentinel 1	Daily	January 2015-now	Europe	1 km	C-band (5.405 GHz)	Copernicus Global Land Service
SMOS L4	Daily	June 2010-now	Europe	1 km	L-band (1.4 GHz)	Barcelona Expert Center
SMAP L3E	Daily	March 2015-now	Globe	9 km	L-band (1.41 GHz)	NASA National Snow and Ice Data Center
SMAP L4	3-hourly	March 2015-now	Globe	9 km	L-band (1.41 GHz)	NASA National Snow and Ice Data Center
Sentinel 1/SMAP combined	Daily	April 2015-now	Globe	3 km	L/C-band	NASA National Snow and Ice Data Center
ASCAT (H115)	Daily	January 2007–December 2018	Globe	12.5 km	C-band (5.255 GHz)	EUMETSAT Satellite Application Facility on Support to Operational Hydrology and Water Management (H SAF)

been tested to demonstrate the feasibility of retrieving soil moisture with Sentinel 1 SAR data (e.g., Alexakis et al., 2017; Bauer-Marschallinger et al., 2018; El Hajj et al., 2017; Gao et al., 2017; Mattia et al., 2017). Among them, Bauer-Marschallinger et al. (2018) adapted the change detection method to estimate global soil moisture at 1 km spatial resolution based on radiometrically calibrated and geo-corrected Sentinel 1 backscatter data. Currently, their method has been applied to deliver daily 1 km soil moisture in an operational manner for the whole of Europe. The Sentinel 1 (version 1) product is available from January 2015 until present, and is disseminated by the Copernicus Global Land Service (<https://land.copernicus.eu/global/products/ssm>).

2.1.2. SMOS L4

The SMOS is an ESA satellite mission that was specifically designed to provide soil moisture and sea surface salinity with a L-band (1.4 GHz) radiometer. After the successful launch in November 2009, SMOS has provided more than 10 years global fully polarized multi-angular observations at both ascending (6:00 a.m. local time) and descending (6:00 p.m. local time) orbit (e.g., Alexakis et al., 2017; Bauer-Marschallinger et al., 2018; El Hajj et al., 2017; Gao et al., 2017; Mattia et al., 2017). The original spatial resolution of retrieved global SMOS soil moisture is around 40 km, which is too coarse for regional applications. A downscaled high-resolution SMOS L4 product covering Europe was therefore developed and released by the Barcelona Expert Center (BEC) (Portal et al., 2020; Piles et al., 2015). This product has spatial resolution of 1 km and is based on the universal triangle concept to merge together the SMOS brightness temperature, SMOS coarse resolution soil moisture, MODIS Normalized difference vegetation index (NDVI) and European Centre for Medium-Range Weather Forecasts (ECMWF) temperature (Kerr et al., 2010). The SMOS L4 (version 5) 1 km soil moisture product is available from the Barcelona Expert Center (<http://bec.icm.csic.es>). In this study, the ascending and descending SMOS L4 soil moisture are simply averaged to get daily SMOS L4 soil moisture.

2.1.3. SMAP L3E and SMAP L4

The SMAP satellite is the second L-band mission from NASA, aiming to monitor global land soil moisture and freeze/thaw state. It was launched in January 2015 and carries both radar (1.26 GHz) and radiometer (1.41 GHz) to respectively provide observations at about 3 km and 40 km spatial resolution with 40° constant incidence angle (Piles et al., 2015; Portal et al., 2020; Portal et al., 2018). Owing to the failure of the radar's power supply in early 2015, only the radiometer can operate and deliver observations from 2015 until now. Different levels of soil moisture products have been developed and distributed by the SMAP mission. These products include swath-based SMAP L2, daily composite SMAP L3, and model assimilated SMAP L4 (Entekhabi et al., 2010). The SMAP soil moisture used in this study is the enhanced SMAP L3 (SMAP L3E) global daily 9 km soil moisture, which is derived from the SMAP interpolated brightness temperature using the Backus-Gilbert optimal interpolation technique (Colliander et al., 2017). The SMAP L3E (version 3) soil moisture is downloaded from the NASA National Snow and Ice Data Center (NSIDC) (https://nsidc.org/data/SPL3SMP_E/v

ersions/3). Similar to SMOS, the SMAP L3E soil moisture at ascending (6:00 p.m. local time) and descending (6:00 a.m. local time) modes are simply averaged to obtain daily soil moisture in this study. The SMAP L4 product is produced based on the assimilation of brightness temperature into the land surface model to improve soil moisture estimates (Reichle et al., 2017a; Reichle et al., 2017b). In the present study, SMAP L4 Global 3-hourly 9 km EASE-Grid Surface (0–5 cm) volumetric soil moisture (version 5) is used, which is available from NSIDC (<https://nsidc.org/data/SPL4SMGP/versions/5>).

2.1.4. SMAP/sentinel 1 combined soil moisture

One of the objectives of SMAP mission is to deliver global 9 km soil moisture from the downscaled radiometer brightness temperature with the use of radar backscatter measurement (O'Neill et al., 2016). However, the failure of SMAP radar hampers the SMAP mission to generate a high-resolution soil moisture product. The Sentinel 1 SAR data were found to be suitable for the fusion with SMAP radiometer. Based on the SMAP/Sentinel active-passive retrieval algorithm (Entekhabi et al., 2010), the SMAP team recently released the global SMAP/Sentinel 1 active-passive high-resolution surface soil moisture product with 3 km spatial resolution (Das et al., 2013; Jagdhuber et al., 2019). This SMAP/Sentinel 1 (version 3) combined product is available from April 2015 to the present, and can be downloaded from the NSIDC (https://nsidc.org/data/spl2smap_s).

2.1.5. ASCAT

The Advanced Scatterometer (ASCAT), on board the Metop-A, Metop-B and Metop-C satellite, operates at the C band (5.255 GHz) in vertical polarization and provides observations at around 25 km and 50 km spatial resolution in both descending (9:30 am) and ascending (9:30 pm) nodes. The change detection algorithm developed by the Vienna University of Technology has been applied to derive soil moisture from the ASCAT backscatter measurements (Wagner et al., 1999). In this study, we use the surface soil moisture Climate Data Record H115 produced by the EUMETSAT Satellite Application Facility on Support to Operational Hydrology and Water Management (H SAF, <http://hsaf.meteoam.it>). Same as Sentinel 1 soil moisture product, it is relative soil moisture represented by degree of saturation ranging from 0% to 100%. The product covers the period from January 2007 to December 2018 with a spatial sampling of 12.5 km.

2.2. JULES-CHESS simulation

The Joint UK Land Environment Simulator (JULES) is a community land surface model that integrates a full suite of land surface process (e.g., water and energy balance, carbon cycle, dynamic vegetation) and allows the interaction between these processes to be investigated. JULES can be run as a standalone model, and is also the land surface component of the next generation UK Earth System Model (UKESM). A detailed model description is given by Best et al. (2011) and Clark et al. (2011). In order to better assess the water, energy and carbon budgets of UK, long-term high-resolution JULES simulation is generated driven with the

Climate Hydrology and Ecology research Support System meteorology (CHES-met) dataset, which includes 1 km resolution gridded meteorological variables over the UK (Robinson et al., 2017). The JULES-CHES model was used to simulate water, carbon and energy fluxes mainly including evaporation, soil moisture, runoff, surface temperature, snow mass, plant respiration, and net gross primary productivities at both daily and monthly scale, beginning in 1961 (Blyth et al., 2019; Martínez-de la Torre et al., 2018). The model configuration, including ancillary files, science options and parameters, is described in Blyth et al. (2019). The land cover data were derived from the CEH Land Cover Map 2000 (Fuller et al., 2002). Canopy heights were set to constant values for each PFT, which were globally representative, except C3 grass which was reduced to better represent UK grassland. The JULES-CHES configuration uses the van Genuchten approach to solve the Darcy Richards equation (Van Genuchten, 1980). The soil parameters were derived from the soil textures given by the Harmonized World Soil Database, using texture classes (Wösten et al., 1999). JULES-CHES used the Probability Distribution Model (PDM) for saturation excess runoff, with parameters dependent on terrain slope (Martínez-de la Torre et al., 2019). The slope was derived from the CEH-IHDTM (Morris and Flavin, 1994). The hydrological cycle of JULES-CHES has been evaluated against country-scale observed river flows and observation-based evaporation products, and site-scale latent and sensible heat fluxes (Blyth et al., 2019). Recent work has evaluated the ability of JULES to model soil moisture in the UK against satellite and COSMOS data, albeit with different pedotransfer functions (Pinnington et al., 2020) and with different driving data and soil physics (Cooper et al., 2020). The JULES-CHES data can be downloaded from the Environmental Information Data Centre (EIDC; <https://catalogue.ceh.ac.uk/documents/c76096d6-45d4-4a69-a310-4c67f8dcf096>). The JULES-CHES simulated soil moisture in the top layer, which is 10 cm thick, from 2015 to 2017 is used in the present study. It is noted that the modeled soil moisture has different depth from that of satellite-based estimates. As stated by Pinnington et al. (2020), the differences between JULES simulated soil moisture at 5 cm and at 10 cm are marginal. Similar results have been reported by previous studies such as Shellito et al. (2018) and Shellito et al. (2020). Therefore, the default JULES top layer (10 cm) soil moisture is directly used to compare and merge with satellite-based soil moisture.

2.3. COSMOS-UK measurements

The Cosmic-ray Soil Moisture Observing System (COSMOS) measures soil moisture based on the theory that the neutrons derived from cosmic rays are attenuated by water present in soil. A detailed description of COSMOS is provided by Zreda et al. (2012) and Evans et al. (2016). In 2013, COSMOS-UK was established by UKCEH to provide near-real time soil moisture measurements from an intensive network of COSMOS stations across the UK. There are currently 51 stations installed and the COSMOS-UK network is likely to expand in future. Each station is equipped with various sensors to measure not only cosmic-ray neutron counts but also other hydro-meteorological variables. Volumetric soil moisture is derived from corrected neutron counts based on site-specific field calibration (Cooper et al., 2021; Evans et al., 2016; Franz et al., 2013). Hourly and daily volumetric soil moisture data from 2013 to 2017 for 46 COSMOS-UK stations are freely available from the COSMOS-UK website (<https://cosmos.ceh.ac.uk>) (Cooper et al., 2021). Fig. 1 shows the locations of 38 sites that are used in this study. These sites are selected because they are located in the UK mainland and were installed before 2017. Details of these sites are provided in Appendix Table A1. On the basis of Köhli et al. (2015), it is estimated that the COSMOS vertical sensing depth, for 86% response, is around 20 cm for typical soil moisture content in the UK ($0.03 \text{ m}^3/\text{m}^3$), while the radial footprint is around 150–200 m. However, as the sensitivity decays exponentially with depth, it has been estimated that on average (over a year), for some typical COSMOS-UK sites, the first 50% of the response is

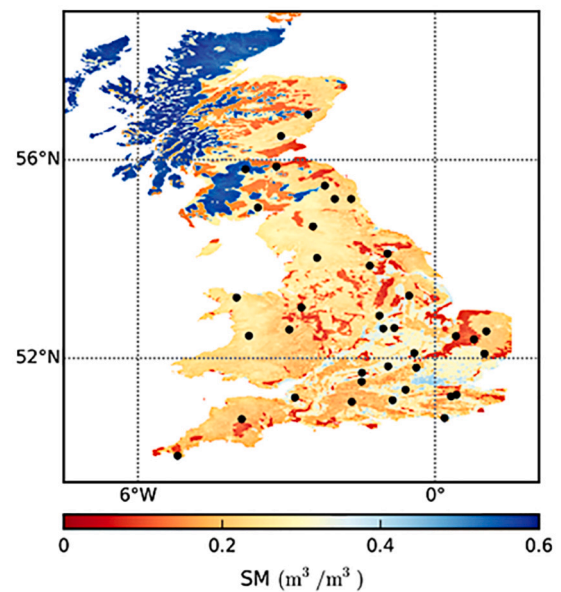


Fig. 1. Distributions of 38 COSMOS-UK stations used in this study. The base map is the spatial pattern of simulated soil moisture from JULES-CHES on 2015.04.22.

from the top 10 cm soil layer (Beale et al., 2021).

3. Methods

All the data products used in this study were aggregated to daily temporal resolution and a subset was taken to cover the UK mainland from 2015.04.01 to 2017.10.12. The evaluation strategy, statistical scores, and merging scheme are described in the following sub-sections.

3.1. Evaluation strategy

3.1.1. Direct comparison with in-situ measurements

For the direct comparison between COSMOS-UK measurements and satellite-based or model-simulated soil moisture, two approaches are applied. One approach uses all available soil moisture values for each product during the study period 2015–2017, while the other is based on collocated measurements that have common dates for all products. The evaluation based on all available measurements can provide the actual accuracy for each product. Using common dates between different products is necessary for a fair comparison of different products. These two approaches can also help to investigate the influence of data sample size on the evaluation. It is noted that all soil moisture products are given in volumetric units (m^3/m^3), except Sentinel 1 and ASCAT whose unit is degree of saturation. To facilitate the comparison, we converted the Sentinel 1 and ASCAT soil moisture to volumetric soil moisture based on the soil porosity information extracted from the Harmonized World Soil Database (HWSD) (Dorigo et al., 2017; Reynolds et al., 2000).

In addition to direct comparison of absolute soil moisture values, soil moisture anomalies were calculated to remove the impacts of seasonal variability on the evaluation. The comparison of soil moisture anomalies can also reduce the representative errors caused by the mismatch of measured soil depth and footprint between COSMOS-UK and satellite or JULES-CHES soil moisture (Albergel et al., 2012; Gruber et al., 2020). The anomaly was calculated with the following equation (Gruber et al., 2013; Peng et al., 2015).

$$Anom_t = SM_t - \overline{SM_w} \quad (1)$$

Where $Anom_t$ is the soil moisture anomaly, SM_t is the soil moisture at day t , and $\overline{SM_w}$ refers to the temporal mean soil moisture over the

moving window of 35 days. The anomaly is calculated only when the soil moisture sample size within the moving window is larger than 6. The use of a 35-day moving window has been suggested in previous soil moisture evaluation studies (Al-Yaari et al., 2019; Albergel et al., 2012; Gruber et al., 2020) to calculate short-term soil moisture anomaly.

Three statistical metrics that have been widely adopted in the soil moisture community, namely Pearson correlation coefficient (R), Bias, and unbiased Root Mean Square Difference (ubRMSD) are used to quantify the differences between each soil moisture product and the COSMOS-UK measurements. These metrics are defined as follows:

$$R = \frac{\text{cov}(SM_{\text{Product}}, SM_{\text{COSMOS}})}{\sigma_{\text{Product}} \sigma_{\text{COSMOS}}} \quad (2)$$

$$\text{Bias} = \overline{SM_{\text{Product}}} - \overline{SM_{\text{COSMOS}}} \quad (3)$$

$$\text{ubRMSD} = \sqrt{\left(\overline{(SM_{\text{Product}} - \overline{SM_{\text{Product}}})^2} + \overline{(SM_{\text{COSMOS}} - \overline{SM_{\text{COSMOS}}})^2} - 2 \overline{(SM_{\text{Product}} - \overline{SM_{\text{Product}}})(SM_{\text{COSMOS}} - \overline{SM_{\text{COSMOS}}})} \right)} \quad (4)$$

Where SM_{Product} is the soil moisture dataset to be evaluated, SM_{COSMOS} is the COSMOS-UK reference soil moisture. Cov is the covariance of both soil moisture time period, while σ_{Product} and σ_{COSMOS} are the standard deviations of the soil moisture period. The overbar in each equation indicates the temporal mean of entire time period.

3.1.2. Evaluation with triple collocation analysis

Furthermore, the method of triple collocation (TC) is applied in this study to estimate the random error variances of the satellite-based products. In contrast to direct comparison with ground-based reference data, the TC-based analysis provides an additional way to quantify errors without knowing the truth. The implementation of TC method needs three independent measurements of soil moisture. Moreover, a few assumptions are required by the TC method (Chen et al., 2018; Gebler et al., 2017): 1) the three measurements are linearly related to the true soil moisture; 2) there is no correlation between errors and the true soil moisture; 3) the errors of the three measurements are independent; 4) the signal and error statistics are stationary. If these assumptions are met, the absolute error standard deviation for each measurement is given as:

$$\begin{aligned} \sigma_{\varepsilon_X} &= \sqrt{\left| \sigma_X^2 - \frac{\sigma_{XY}\sigma_{XZ}}{\sigma_{YZ}} \right|} \\ \sigma_{\varepsilon_Y} &= \sqrt{\left| \sigma_Y^2 - \frac{\sigma_{YX}\sigma_{YZ}}{\sigma_{XZ}} \right|} \\ \sigma_{\varepsilon_Z} &= \sqrt{\left| \sigma_Z^2 - \frac{\sigma_{ZX}\sigma_{ZY}}{\sigma_{XY}} \right|} \end{aligned} \quad (5)$$

Where σ_i^2 refers to the variances of measurements X, Y and Z, and σ_{ij} is the covariance of the measurements. Details of the derivation can be found in (Gruber et al., 2016). Another measure is the signal-to-noise ratio (SNR), which is given in decibel units (dB) and is calculated as:

$$\begin{aligned} \text{SNR}_X &= -10 \log \left(\frac{\sigma_X^2 \sigma_{YZ}}{\sigma_{XY} \sigma_{XZ}} - 1 \right) \\ \text{SNR}_Y &= -10 \log \left(\frac{\sigma_Y^2 \sigma_{XZ}}{\sigma_{YX} \sigma_{YZ}} - 1 \right) \\ \text{SNR}_Z &= -10 \log \left(\frac{\sigma_Z^2 \sigma_{XY}}{\sigma_{ZX} \sigma_{ZY}} - 1 \right) \end{aligned} \quad (6)$$

In this study, X is the COSMOS-UK soil moisture, Y is one of the satellite-based soil moisture products, and Z is the JULES-CHESS simulated soil moisture. As suggested by previous studies such as Gruber et al. (2016) and Al-Yaari et al. (2014), the error statistics are calculated

only when temporally and spatially collocated triplets have at least 100 measurements. The TC analysis is performed for both original soil moisture and anomalies at all COSMOS-UK stations. It is noted that the TC analysis here aims to provide a relevant evaluation of the performance of different satellite-based soil moisture products at the COSMOS site scale.

3.2. Merging scheme

Merging different soil moisture products is advantageous because it minimizes random retrieval errors. The current study applies a least-squares merging scheme to obtain optimal estimates of soil moisture over the UK mainland. The least squares framework can be described as (Yilmaz et al., 2012):

$$SM_{\text{merged}} = w_X SM_X + w_Y SM_Y + w_Z SM_Z \quad (7)$$

Where SM_{merged} is the merged soil moisture, SM_i is the individual soil moisture product, and w_i is the weight that is assigned to each product. The weights are calculated to minimize the random errors in the merged product. The weights are decided by the error variances and covariances of the soil moisture products (Gruber et al., 2019b). As stated in the previous section, the TC method is an effective way to estimate random error variances. It can also be used to derive relative rescaling factors that will match the variability of different products to a common data space. For example, taking product X as the reference, then the scaling factors can be calculated as (Gruber et al., 2016):

$$\begin{aligned} \beta_X &= 1 \\ \beta_Y &= \frac{\sigma_{XZ}}{\sigma_{YZ}} \\ \beta_Z &= \frac{\sigma_{XY}}{\sigma_{ZY}} \end{aligned} \quad (8)$$

Where β_i is the scaling factor for each product and is determined by error covariances. Clearly, β_X is set to 1 due to its serving as the reference. Then the products Y and Z are rescaled using the following equations (Gruber et al., 2017; Gruber et al., 2016):

$$\begin{aligned} Y_{\text{rescaled}} &= \beta_Y * (Y - \bar{Y}) + \bar{X} \\ Z_{\text{rescaled}} &= \beta_Z * (Z - \bar{Z}) + \bar{X} \end{aligned} \quad (9)$$

Where \bar{X} , \bar{Y} and \bar{Z} are the temporal mean of X, Y and Z respectively. The weight w_i of each product is then derived as follows (Gruber et al., 2017; Zeng et al., 2016):

$$\begin{aligned} w_X &= \frac{\sigma_Y^2 \sigma_Z^2}{\sigma_X^2 \sigma_Y^2 + \sigma_X^2 \sigma_Z^2 + \sigma_Y^2 \sigma_Z^2} \\ w_Y &= \frac{\sigma_X^2 \sigma_Z^2}{\sigma_X^2 \sigma_Y^2 + \sigma_X^2 \sigma_Z^2 + \sigma_Y^2 \sigma_Z^2} \\ w_Z &= \frac{\sigma_X^2 \sigma_Y^2}{\sigma_X^2 \sigma_Y^2 + \sigma_X^2 \sigma_Z^2 + \sigma_Y^2 \sigma_Z^2} \end{aligned} \quad (10)$$

For collocated triplets, the above formula is used to estimate weights from the rescaled products and merge the rescaled products based on eq. 7. In order to increase the data coverage of the merged product, a merging scheme proposed by Gruber et al. (2017) based on the one-tailed Pearson's correlation significance is applied for the non-collocated samples. TC weighted merging is applied if p -value is less than 0.05 among the three products. Where only two datasets are available, the least-squared-based weights are derived from the uncertainties and a weighted average between the two products is used for merging. Table 2 details the alternative methods used if TC merging is rejected, including the decision on whether to use one product, the arithmetic mean of two

Table 2

Merging scheme for non-located grids. X, Y, and Z refer to different soil moisture products.

p-value <0.05 (X-Y)	p-value <0.05 (X-Z)	p-value <0.05 (Y-Z)	Merging scheme
yes	yes	yes	TCA weighted mean(X, Y, Z) ^a
yes	yes	no	X
no	yes	yes	Z
yes	no	yes	Y
yes	no	no	Arithmetic mean (X, Y)
no	yes	no	Arithmetic mean (X, Z)
no	no	yes	Arithmetic mean (Y, Z)
no	no	no	Disregard

^a where only two datasets are available, the least-squared-based weights are derived from the uncertainties and a weighted average between the two products is used in the merging.

products, or to disregard the pixel. This simple averaging scheme might become problematic if one product is well sampled in time but with significantly low quality. The use of this product to fill the gaps of higher quality dataset may reduce the overall quality of the merged time series. However, improved soil moisture temporal coverage is preferable to absolute quality for many applications such as drought monitoring and runoff simulation. Therefore, this simple averaging scheme is used in order to provide the highest possible sample density. In the present study, SMAP L3E and JULES-CHESS are firstly resampled to 12.5 km spatial resolution and then merged together with ASCAT using the proposed scheme.

4. Results and discussion

4.1. Comparison with all available observations

Fig. 2 shows the error statistics for satellite-based and JULES-CHESS soil moisture compared to COSMOS-UK observations at 38 stations. Note that the data sample size for each product might be different because for each individual product all available observations between April 2015 and October 2017 are used. For most stations, the SMAP L3E and JULES-CHESS outperform other soil moisture products with higher R and lower ubRMSD values. There is a large variation in the error scores over different stations for all the products. Relatively low R values are found at stations GLENS, HARWD, RDMER, TADHM for all the products. This is because all these locations have organic soils and low bulk density. There are still large uncertainties in retrieving soil moisture from organic soils via satellite microwave signals. Specifically, the surface roughness and vegetation parameters used in the radiative transfer model normally only account for mineral soils and are not properly calibrated over organic soils (Jonard et al., 2018; Peng et al., 2021). The

results suggest the importance of deriving specific roughness and vegetation parameters for the improvement of microwave soil moisture products over surfaces with organic soil. The JULES model simulation also has large uncertainties over organic soils, due to its limitation in representation of organic soil process in the current model structure. In addition, the COSMOS measured soil moisture also has certain uncertainties in organic soil, where organic matter contains hydrogen and has strong impacts on measured COSMOS soil moisture particularly for wet soil in winter months. Generally negative Bias are found for all products, which is likely due to the vertical depth mismatch between COSMOS and other products. There are no simple approaches to calibrate all these products to represent the same depth. One way to make a fair comparison is to use COSMOS data to calibrate hydrological models (e.g. Hydrus) at COSMOS sites. The first layer soil moisture can then be extracted from the model and compared with satellite-based products.

In order to have a general view of the performance of different products, Fig. 3 summarizes the statistical scores for all stations with box plots. It is shown that the JULES-CHESS soil moisture has the best performance with median R of 0.85, median ubRMSD of 0.041 m³/m³. The SMAP L3E has similar median ubRMSD (0.048 m³/m³) and median R (0.76) compared to SMAP L4 (ubRMSD = 0.046 m³/m³, R = 0.71). The other products have relatively high ubRMSD values larger than 0.062 m³/m³. Since the SMOS L4 is a downscaled soil moisture product, the bias is attributed to the downscaling method and the input data such as original SMOS product and MODIS NDVI product (Piles et al., 2011). The accuracy of SMOS soil moisture is also highly influenced by the impacts of Radio Frequency Interference (RFI) compared to SMAP, which has an improved technology for RFI filtering (Entekhabi et al., 2010). For Sentinel 1 and ASCAT, the large difference might be caused by uncertainties introduced during the conversion of relative soil moisture unit into volumetric soil moisture, which relies on the coarse soil porosity data derived from the HWSO soil texture (Wagner et al., 2013). High-quality and high-resolution soil porosity data is therefore required to improve the accuracy of Sentinel 1 and ASCAT volumetric soil moisture. In addition, the impacts of dynamic vegetation are not accounted for in the current Sentinel 1 product and the improvement of the algorithm with dynamic vegetation correction is expected to boost the quality (Al-Yaari et al., 2014; Bauer-Marschallinger et al., 2018).

The results for the comparison of soil moisture anomalies are summarized in Figs. 4 and 5. Compared to absolute soil moisture, the R values for anomalies drop significantly for all the products (with median R ranging from 0.25 to 0.73, Fig. 5). This is attributed to the removal of seasonal cycle that contributes to the strong correlation for absolute soil moisture comparison (Al-Yaari et al., 2019; Peng et al., 2015). Due to the decrease of soil moisture magnitude, the ubRMSD for anomalies also diminish for all the products. The smallest ubRMSD is found for JULES-CHESS (0.021 m³/m³), followed by SMAP L4 (0.024 m³/m³), SMAP L3E (0.033 m³/m³), SMOS L4 (0.047 m³/m³), ASCAT (0.055 m³/m³),

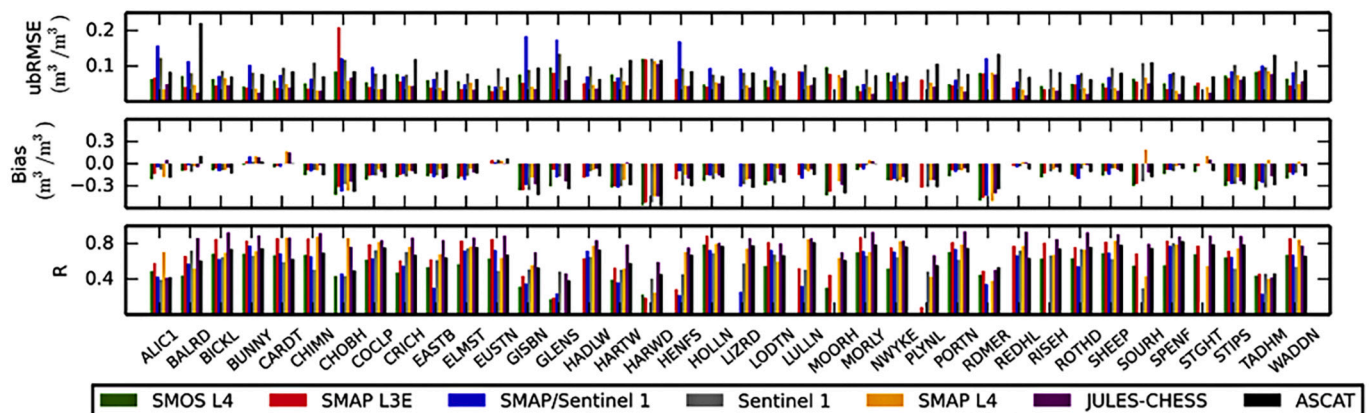


Fig. 2. Statistical scores for the direct comparison between all soil moisture products against COSMOS-UK measurements from April 2015 to October 2017.

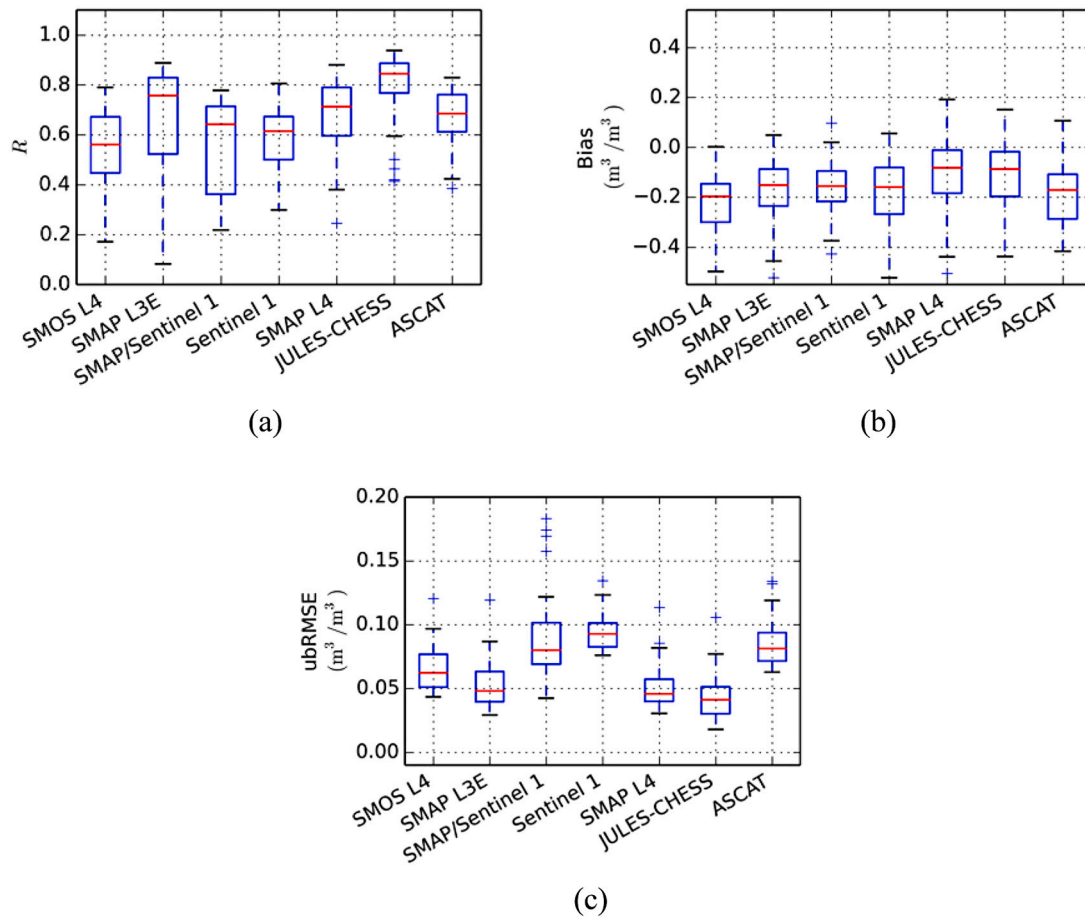


Fig. 3. Box plots of the statistical scores for direct comparison of absolute soil moisture at 38 COSMOS-UK stations: (a) R ; (b) Bias; (c) ubRMSE.

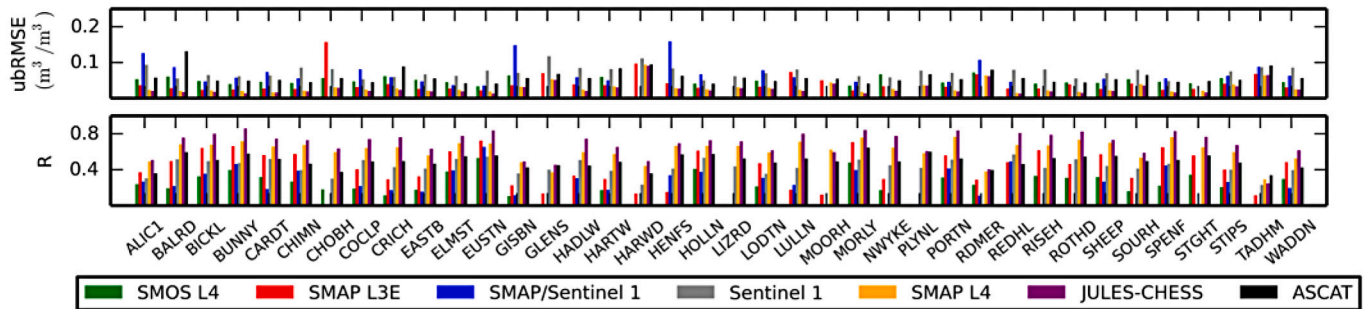


Fig. 4. Statistical scores for the comparison of soil moisture anomalies from April 2015 to October 2017.

SMAP/Sentinel 1 ($0.059 \text{ m}^3/\text{m}^3$), and Sentinel 1 ($0.071 \text{ m}^3/\text{m}^3$). Therefore, this comparison of anomalies generally shows similar results to the absolute soil moisture comparison, highlighting the relatively better performance of JULES-CHESS and SMAP (L3E and L4) soil moisture products.

4.2. Comparison based on temporal collocated observations

In order to make a relative fair comparison between all the products, the analysis is limited to temporal collocated dates for different products. Appendix Fig. A1 presents the evaluation scores for absolute soil moisture, while the results for anomalies are summarized in Fig. A2. Generally, it can be seen that the evaluation scores here are different from the results shown in Figs. 3 and 5, which is due to different sample dates that are considered in comparisons either for all available

observations or for observations only on common dates. The performance of all the products are better for common dates than all available dates with higher median R and lower median ubRMSE values. The improvement in the magnitudes of statistical scores is higher for absolute values comparisons than anomaly comparisons. This may be because that the reduced sample size can represent a complete seasonal variation. In addition, the temporal collocated samples might potentially remove low quality data for all products, which is caused by different quality flag standards in each product. In terms of the ranking for all products, it is the same as the results from all available observations, with better performance found for JULES-CHESS, SMAP L3E and SMAP L4, followed by ASCAT, SMOS L4, SMAP/Sentinel 1, and Sentinel 1. Specifically, the SMAP L3E and JULES-CHESS respectively have median ubRMSE of $0.042 \text{ m}^3/\text{m}^3$ and $0.039 \text{ m}^3/\text{m}^3$, which are close to the target accuracy ($0.04 \text{ m}^3/\text{m}^3$) set by the SMAP mission. The

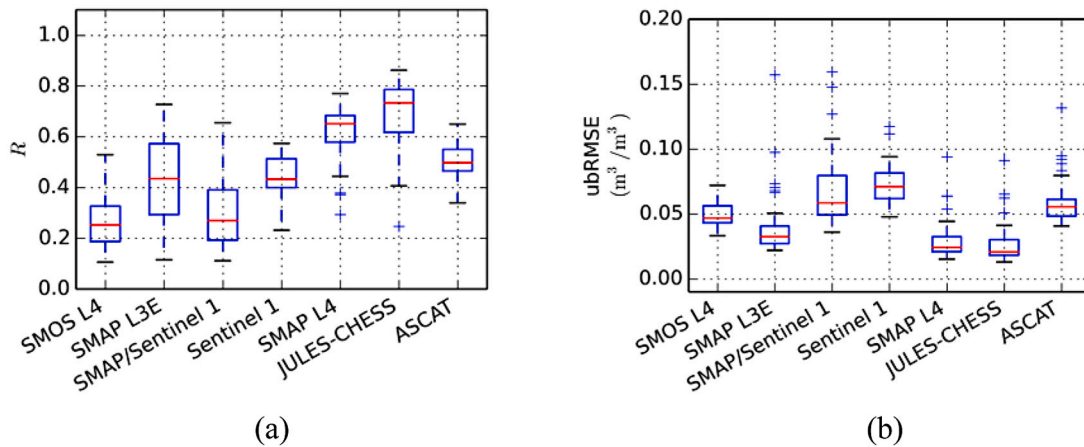


Fig. 5. Box plots of the statistical scores for comparison of soil moisture anomalies at 38 COSMOS-UK stations: (a) R ; (b) ubRMSE.

findings here are in line with the results from previous studies such as Colliander et al. (2017) and Montzka et al. (2017). Although the COSMOS measurements can reduce the representation errors caused by spatial resolution mismatch between the reference and soil moisture products, other sources of uncertainties still exist and contribute to the final evaluation scores (Al Bitar et al., 2017; Gruber et al., 2020). For example, the measured soil depths vary among different techniques, which could lead to different dynamics and responses in the measured soil moisture. In addition, the calibration model used, does not strictly apply to very high soil moisture content, and highly organic soils, thus further work is required to reduce these uncertainties. Therefore, in addition to direct comparison with the COSMOS data, the TC approach is recommended among the soil moisture community as a method for achieving an independent evaluation of satellite-based products without specifying a reference.

4.3. Comparison based on triple collocation

Fig. 6 shows the summary of absolute error standard deviation and SNR for each product calculated based on TC analysis at all COSMOS sites. It is found that the SMAP L3E and SMAP L4 have the best performance with relative low error and high SNR among all the satellite products. Compared to SMAP L3E and SMAP L4, ASCAT and SMOS L4 have worse performance but better performance than SMAP/Sentinel 1 and Sentinel 1. The same ranking of the performance of these products is found for the TC analyses based on absolute soil moisture (Fig. 6) and

anomalies (Appendix Fig. A3). The results obtained here are generally consistent with the direct evaluation presented in Sections 4.1 and 4.2. In addition, similar findings based on triple collocation also highlighted the generally better performance of SMAP L3E compared with other coarse-resolution satellite products (Chen et al., 2018; Montzka et al., 2017). It has been reported that using two passive microwave soil moisture products in the triple collocation analysis is subject to error-correlation, which can lead to unreliable TC estimates (Gruber et al., 2020). Considering the active microwave characteristics of ASCAT and its comparable accuracy with SMOS L4, the SMAP L3E and ASCAT products are selected to merge with JULES-CHESS soil moisture over the British mainland in this study.

4.4. Evaluation of TC merged soil moisture

The weights are estimated based on the error variances of SMAP L3E, ASCAT and JULES-CHESS that are calculated by triple collocation. Low error variances in the triple collocation analysis are assigned relatively high weights, while high error variances indicate low weights. Fig. 7 shows the relative weights that are used to merge the three soil moisture products. Compared with SMAP L3E and JULES-CHESS, ASCAT particularly has relatively higher weights in coastal and northern regions of the British mainland, implying that the merged soil moisture over these parts will be more heavily weighted towards ASCAT than the other products. SMAP L3E has relatively high weights in southeastern regions, while high weights are generally assigned to JULES-CHESS over inland

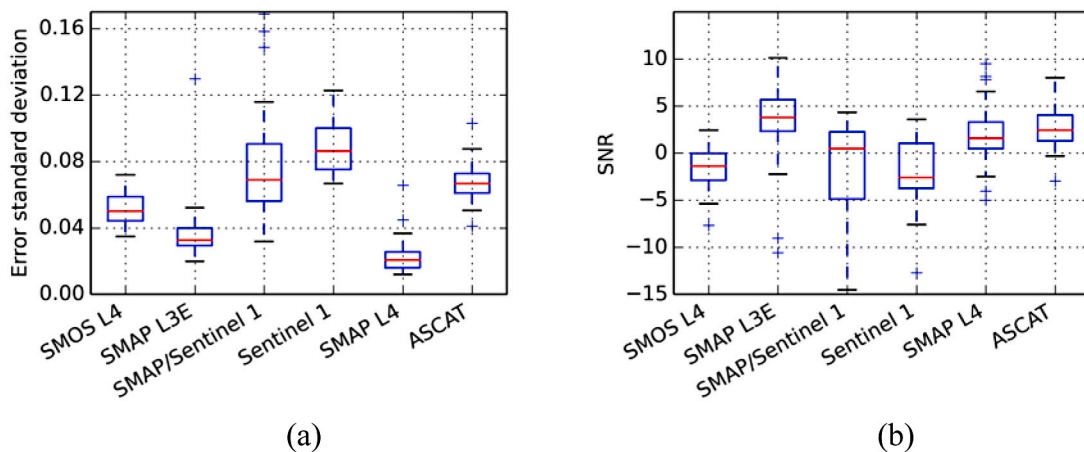


Fig. 6. Box plots of (a) the absolute error standard deviation, and (b) SNR [dB] for each satellite-based product calculated from the triple collocation analysis of absolute soil moisture at all COSMOS sites.

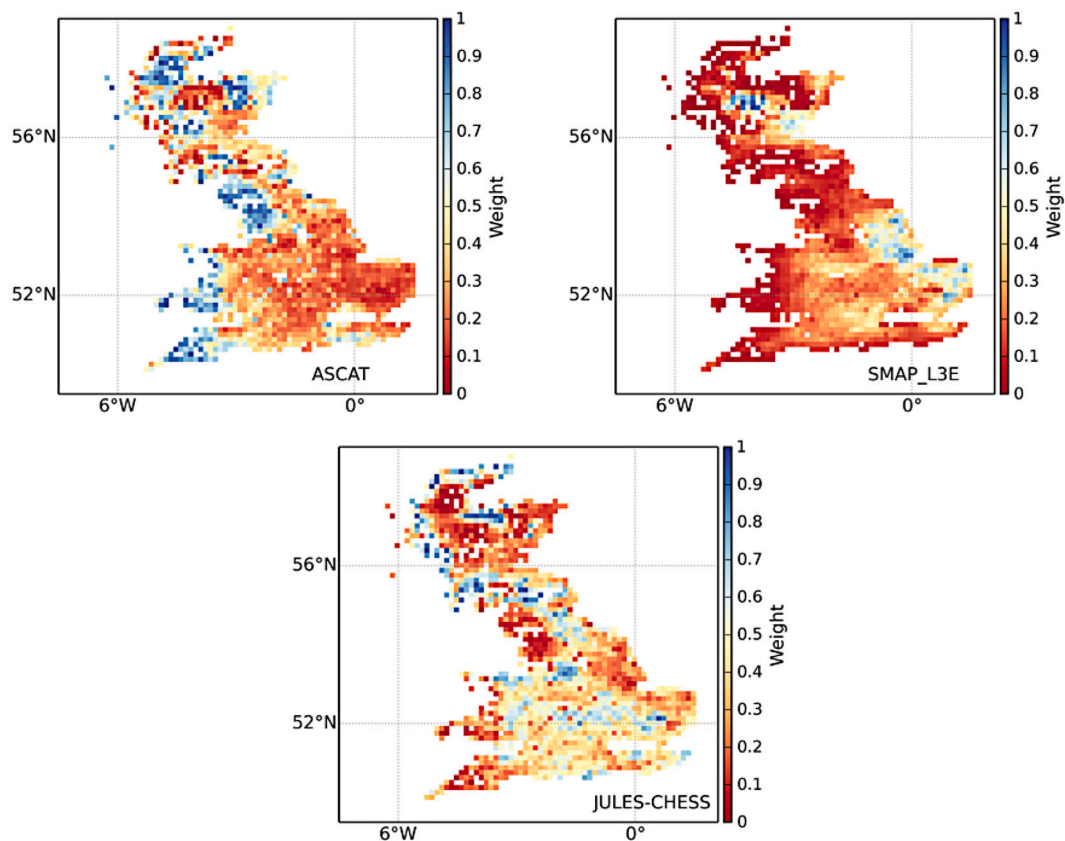


Fig. 7. The soil moisture weights estimated using triple collocation, which are used for merging together the SMAP L3E, ASCAT and JULES-CHESS soil moisture.

areas. Note that the white areas in the maps correspond to non-located pixels, which are merged using the scheme listed in Table 2. Fig. 8 below shows the spatial distribution of the merging method applied in this study. In the vast majority of cases, TC merging was used. The arithmetic mean between two products was very rarely used. The combination of TC merging approach and simple average scheme can increase the data coverage of the merged product. On the other hand, it may cause temporal non-continuity for data points when not all products are available.

It is noted that the merged soil moisture has 12.5 km spatial

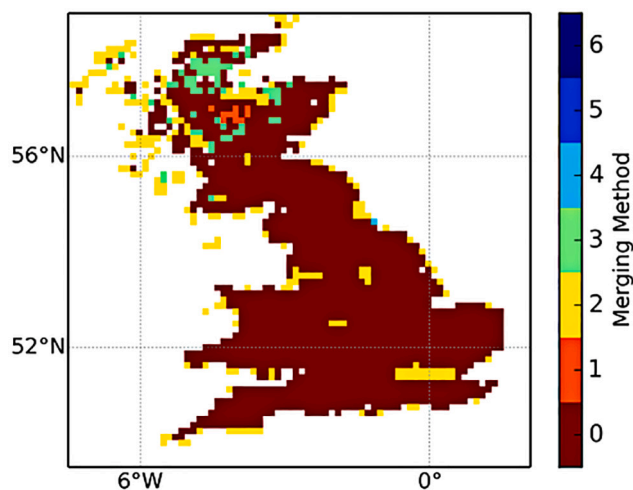


Fig. 8. Map of merging method used. 0 = TCA, 1 = SMAP only, 2 = CHESS only, 3 = ASCAT only, 4 = Arithmetic mean (SMAP, CHESS), 5 = Arithmetic mean (SMAP, ASCAT), 6 = Arithmetic mean (CHESS, ASCAT).

resolution and daily time scale. Fig. 9 shows the spatial patterns of original soil moisture and merged soil moisture for March 2016. It can be seen that the merged product integrates the characteristics of all the original products and should theoretically minimize the random retrieval errors associated with the original products. It is found that the spatial variation is different for all products, but the merged products has similar wet and dry patterns to SMAP L3E, presenting higher levels of soil moisture in northern and southwestern parts of the UK, and a general decrease in wetness in southwestern regions.

In order to evaluate the accuracy of the merged product, we present comparisons of absolute values against independent COSMOS-UK measurements in Fig. 10. Note that the comparison here is based on collocated dates for different products (SMAP L3E, SMAP L4, SMOS L4, ASCAT, JULES-CHESS, Merge). Comparison of the absolute values shows that the merged product and JULES-CHESS have the best error scores in R and ubRMSD compared to other products, with a slightly better performance observed in the median values for merged product ($R = 0.87$, $ubRMSD = 0.038 \text{ m}^3/\text{m}^3$). However, JULES-CHESS and SMAP L4 present lower bias than others, and the merged product has similar bias to SMAP L3E. The same comparison of anomalies was also conducted and the results are shown in Appendix Fig. A4. The performance of anomalies was found to be similar to that of absolute values, with JULES-CHESS and the merged products outperforming other products, but the median R and ubRMSD values for JULES-CHESS were found to be slightly better than the merged product. In order to gain insight into the performance of the original and merged products, the time series of soil moisture over six stations are plotted and explored in Fig. 11. It can be seen that SMAP L3E, ASCAT, and the merged products generally have a greater range of temporal variability compared with JULES-CHESS and SMAP L4. On one hand, this finding suggests that the JULES-CHESS simulation has more muted temporal dynamics, which might be attributed to uncertainties from either the forcing datasets or

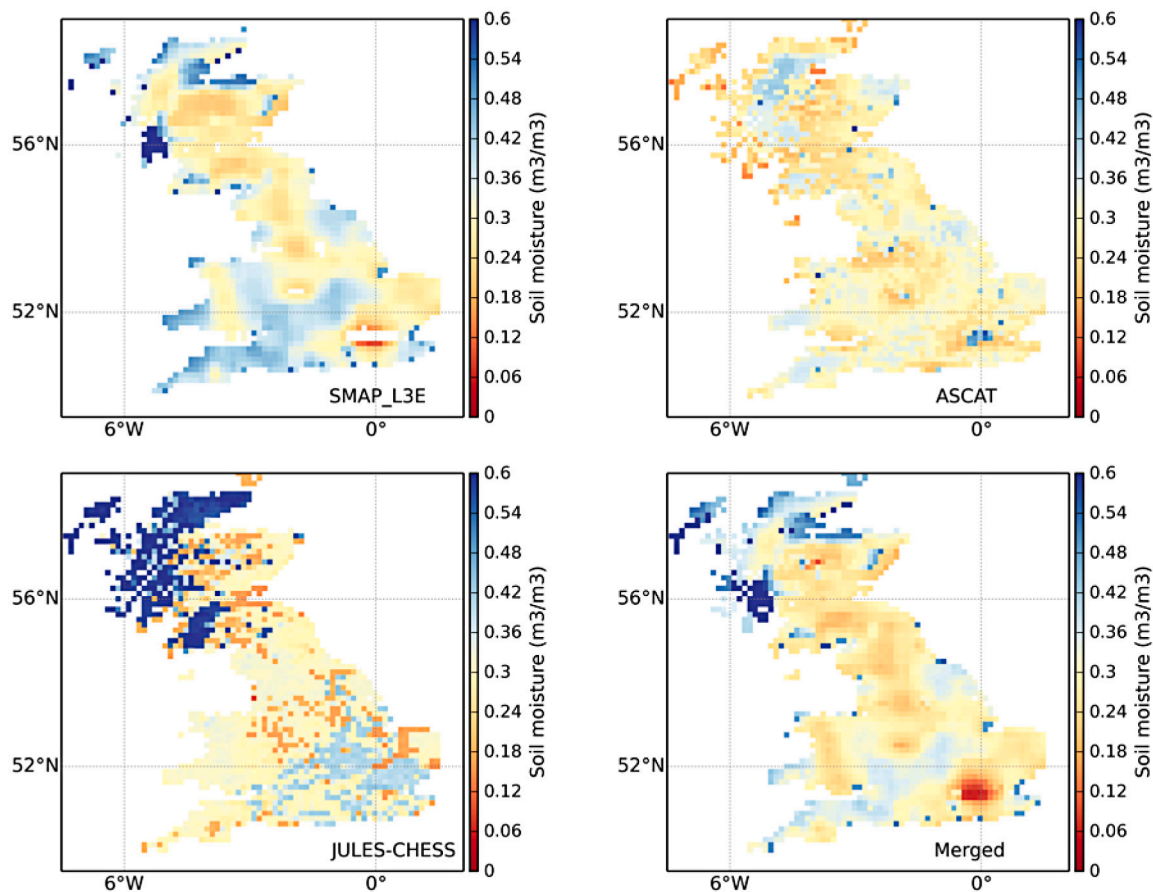


Fig. 9. Comparison of spatial maps between original and merged soil moisture on March 2016.

the JULES model soil parameters. The method of temporal disaggregation in JULES-CHESS uses smoothly varying diurnal cycles and simple disaggregation of rainfall (Williams and Clark, 2014). This may not fully represent sub-daily extremes of both supply (precipitation) and demand (evaporation, calculated from temperature, air pressure, humidity, wind speed and radiation variables) of water into and out of the soil, which may suppress short timescale dynamics. The soil properties, in particular hydraulic conductivity at saturation and soil moisture at saturation, have an effect on both the temporal dynamics of the soil moisture and the overall range that the soil moisture can attain. Recent work with other pedotransfer functions suggests changes to these parameters can improve the temporal dynamics as well as the overall mean (Pinnington et al., 2020; Cooper et al., 2020). On the other hand, the improved temporal dynamics present in the merged product benefits from the integration of information from the satellite soil moisture products. Specifically, in the current study, this improvement results from the rescaling of JULES-CHESS to SMAP L3E, which has similar temporal variability to COSMOS measurements and was used as the reference for TC merging. Similar results have been reported by a recent study that assimilates SMAP data into the JULES model to improve soil moisture prediction (Pinnington et al., 2020). The improved performance of the merged product in the absolute value comparison is due to the minimization of sampling errors associated in parent products. However, the removal of seasonal variability in the anomaly analysis reduces its performance and results in similar error scores compared to JULES-CHESS soil moisture. In addition, it is found that the merged product does not always improve or outperform original products compared to the measurements. For example, large discrepancies between the merged product and COSMOS measurements at sites RDMER and TADHM may be due to the presence of organic soils at these sites. As stated in section 4.1, all products including model simulation, satellite

and COSMOS have large uncertainties over peatland with organic soils. The accuracy of the merged product is also contingent on the reference product during the TC analysis, which is SMAP L3E in this study. If SMAP L3E products have large biases compared to COSMOS measurements, then there might be no improvements of the merged product. In summary, the results presented here highlight the advantages of the merged product, which integrates the desirable characteristics of the component soil moisture products and reduces unwanted random retrieval errors. The TC merging scheme can facilitate the generation of high-quality, temporally and spatially consistent soil moisture information via fusing model simulation and satellite products over the UK mainland. Given the availability of satellite soil moisture products, and the potential for near-real-time JULES-CHESS if the driving datasets are available in a timely manner, this provides a simple way to integrate the advantages of multi-source soil moisture and provide high-quality soil moisture estimates. This would be beneficial for a wide range of applications in climate science, hydrology, ecosystem research and agriculture, along with a range of other sectors.

4.5. Comparison of TC and arithmetic mean merging methods

Fig. 12 shows the comparison between the TC merged product, the simple arithmetic average product, and the JULES-CHESS product. It can be seen from the box plots that all products have similar performance in terms of R, ubRMSD, and bias. For JULES-CHESS and the TC merged product, the results here are almost the same to the comparison shown in Fig. 10. Although slightly worse performance on R and ubRMSD was found for the arithmetic average product compared to JULES-CHESS and the TC merged product, the median bias value of the arithmetic average product is slightly smaller than that of the TC merged product. It suggests that simple averaging also leads to a merged product

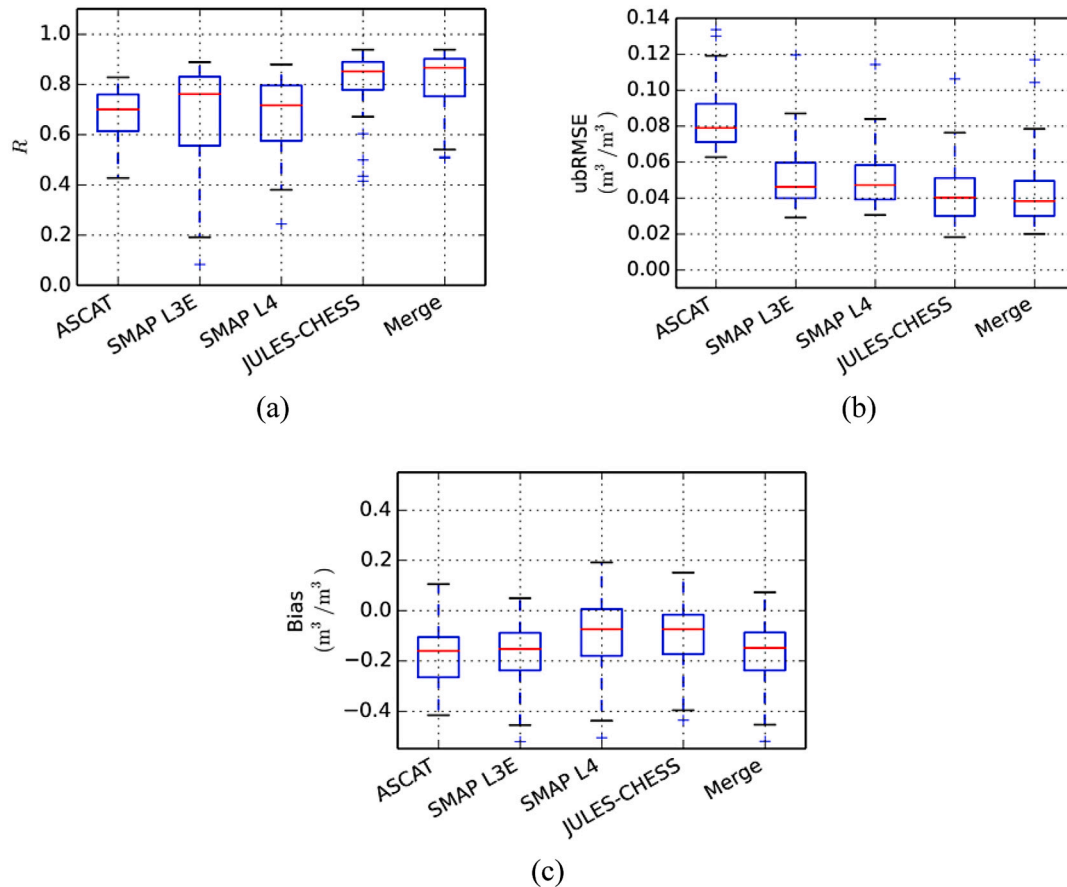


Fig. 10. Evaluation of ASCAT, SMAP L3E, SMAP L4, JULES-CHESS, and merged absolute soil moisture values against independent COSMOS-UK measurements.

with similar performance as the one based on the TC merging approach. Yilmaz et al. (2012) also reported that the TC merging scheme did not always produce a better product than that of simple averaging. Such similarity could be due either to the approximately equal weighting of the three original products or to the optimal TC weighting but small differences among the original products. It further implies that the stationary random error assumption associated with the TC merging approach should be improved to better account for the spatial and temporal non-stationary error (Zhou et al., 2021). Nevertheless, the TC-based approach should be preferred over the simple averaging method, because it can provide optimal weights and would provide a better merged product in areas where the parent products have large differences.

5. Conclusion

High-quality and high-resolution soil moisture information is of significance for various hydrological and meteorological applications in the UK. Currently, there are several soil moisture products available either from satellite retrievals (e.g., SMAP L3E, SMAP L4, SMOS L4, SMAP/Sentinel 1, Sentinel 1, ASCAT) or model simulations (e.g., JULES-CHESS). The aim of this study is to comprehensively evaluate these products and merge the better-performing products together to generate the best soil moisture product for the UK. Direct comparison with COSMOS-UK measurements and independent comparison based on triple collocation were applied to evaluate the quality and consistency of these products. A least-squares merging scheme with error variances estimated by triple collocation was used to merge the different soil moisture products. Several conclusions are drawn from the above analyses.

1. JULES-CHESS and SMAP L3E soil moisture have lower errors compared with other products when compared directly with COSMOS-UK measurements and when evaluated using independent triple collocation. All the products studied here show high errors in organic soils, which suggests that specific roughness and vegetation parameters are required for the improvement of satellite-based soil moisture over surfaces with organic soils. The JULES model also needs to be improved to better simulate soil moisture over organic soils.
2. The COSMOS-UK network provides a valuable reference dataset for the evaluation of satellite and model-based soil moisture products, and reduces footprint representative errors to certain extent. However, the mismatch in soil depth and footprint among different products, as well as COSMOS-UK soil moisture calibration uncertainty particularly over highly organic soils still exist and contribute to the error scores presented in the current study.
3. The TC merged soil moisture dataset presented in this paper integrates the characteristics of the model simulated and satellite-based soil moisture products. In particular, the limited temporal variability of JULES-CHESS simulated soil moisture can be improved in situations where the satellite soil moisture has better temporal dynamics. The TC merging scheme is preferred over simple arithmetic averaging because it provides optimal weighting and the ability to produce a better merge product in areas where there are large differences between the parent products. The stationary error assumption associated with the TC merge scheme should be improved to account for the spatial and temporal non-stationary errors, which would result in improved merging skills.

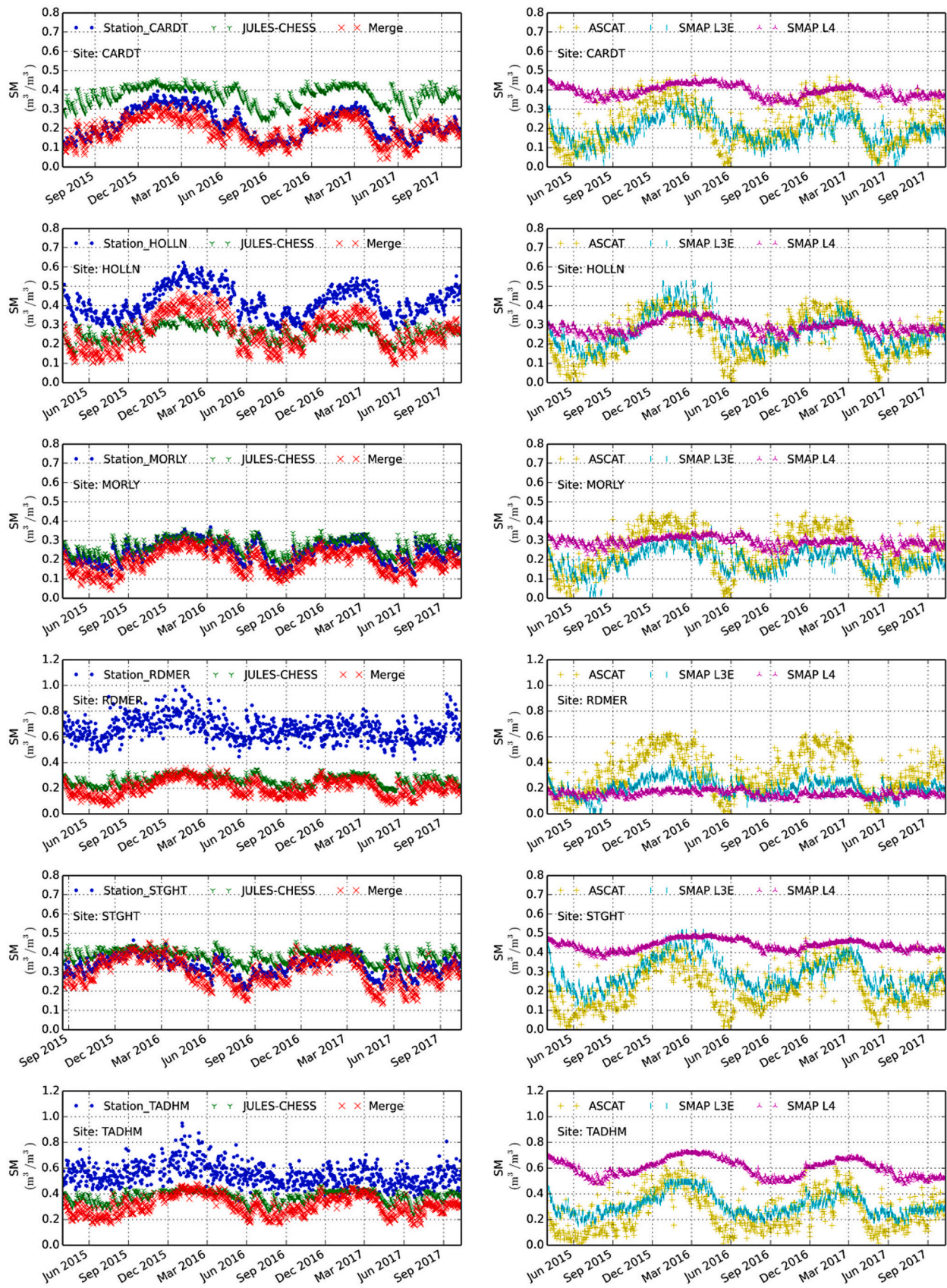


Fig. 11. Time series of the soil moisture from JULES-CHESS and merged soil moisture on the left hand side, and ASCAT, SMAP L3E and SMAP L4 on the right hand side at COSMOS-UK stations distributed over different areas of UK.

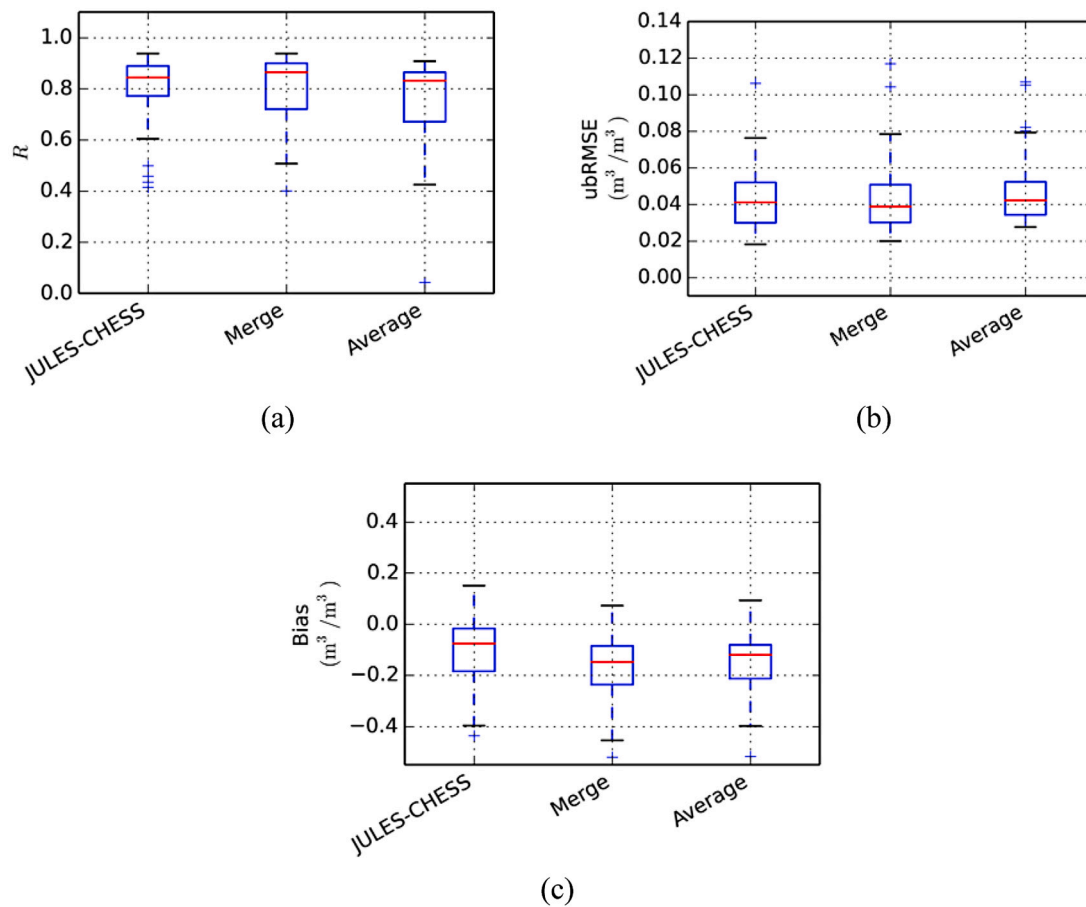


Fig. 12. Box plots of the statistical scores for JULES-CHESS, TC merged and arithmetic average soil moisture compared with COSMOS-UK measurements.

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.

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Appendix A

Table A1

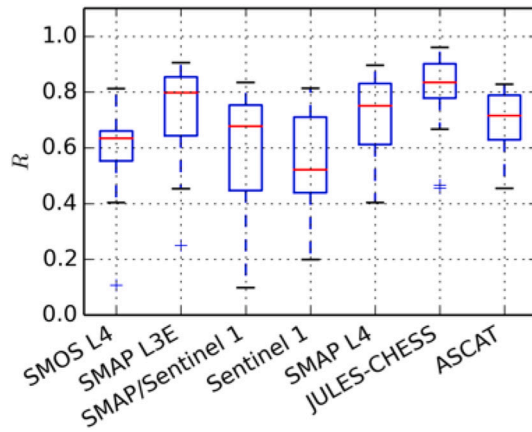
List of the COSMOS-UK stations used in the current study.

Station name	Station ID	Latitude (°)	Longitude (°)	Elevation (m)	Land cover	Start date
Alice Holt	ALIC1	51.154 N	0.858 W	80	Deciduous Broadleaf Forest	6-Mar-15
Balruddery	BALRD	56.482 N	3.112 W	130	Farmland	16-May-14
Bickley Hall	BICKL	53.026 N	2.701 W	78	Improved Grassland	28-Jan-15
Bunny Park	BUNNY	52.861 N	1.127 W	39	Arable	27-Jan-15
Cardington	CARDT	52.106 N	0.425 W	29	Grassland	24-Jun-15
Chimney Meadows	CHIMN	51.708 N	1.479 W	65	Grassland	2-Oct-13
Chobham Common	CHOBH	51.368 N	0.598 W	47	Heath	24-Feb-15
Cockle Park	COCLP	55.216 N	1.694 W	87	Grassland and Arable	21-Nov-14
Crichton	CRICH	55.043 N	3.583 W	42	Grassland	2-Dec-14
Easter Bush	EASTB	55.867 N	3.207 W	208	Grassland	14-Aug-14
Elmsett	ELMST	52.095 N	0.993E	76	Arable	11-Aug-16
Euston	EUSTN	52.336 N	0.796E	18	Improved Grassland	31-Mar-16
Gisburn Forest	GISBN	54.024 N	2.385 W	246	Coniferous Woodland	15-Aug-14
Glensauigh	GLENS	56.914 N	2.562 W	399	Grass and Heather Moorland	14-May-14
Hadlow	HADLW	51.229 N	0.320E	33	Improved Grassland	27-Oct-16
Hartwood Home	HARTW	55.810 N	3.829 W	225	Grassland/ Woodland	20-May-14

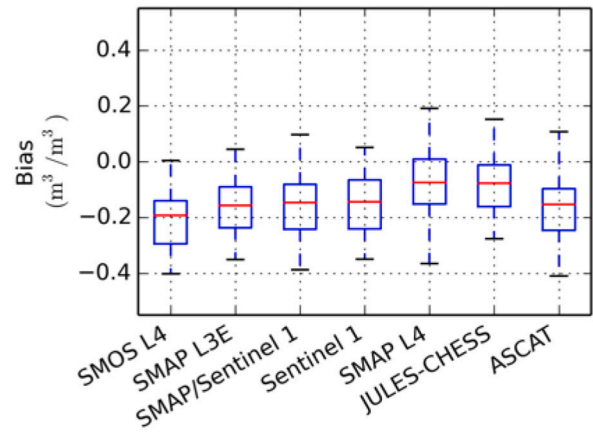
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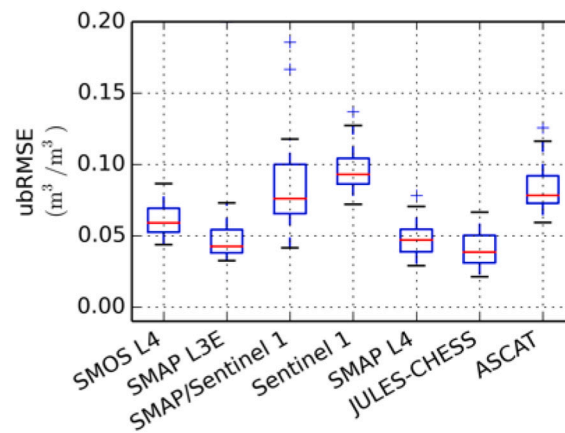
Station name	Station ID	Latitude (°)	Longitude (°)	Elevation (m)	Land cover	Start date
Harwood Forest	HARWD	55.216 N	2.024 W	300	Coniferous Woodland	20-May-15
Henfaes Farm	HENFS	53.225 N	4.012 W	287	Semi-Natural Grassland	17-Dec-15
Hollin Hill	HOLLN	54.111 N	0.960 W	82	Grassland	25-Mar-14
The Lizard	LIZRD	50.033 N	5.200 W	85	Grassland/Heath	17-Oct-14
Loddington	LODTN	52.610 N	0.826 W	186	Arable	26-Apr-16
Lullington Heath	LULLN	50.794 N	0.189E	119	Grassland/Heath	16-Dec-14
Moor House	MOORH	54.659 N	2.468 W	565	Cotton Grass/Heather	4-Dec-14
Morley	MORLY	52.548 N	1.034E	55	Arable	14-May-14
North Wyke	NWYKE	50.774 N	3.906 W	181	Grassland/Pasture	16-Oct-14
Plynlimon	PLYNL	52.453 N	3.763 W	542	Semi-Natural Grassland	5-Nov-14
Porton Down	PORTN	51.120 N	1.681 W	146	Grassland	18-Dec-14
Redmere	RDMER	52.446 N	0.421E	3	Shallow Arable	11-Feb-15
Redhill	REDHL	51.263 N	0.429E	91	Improved Grassland	18-Feb-16
Riseholme	RISEH	53.262 N	0.526 W	53	Improved Grassland	4-May-16
Rothamsted	ROTHD	51.814 N	0.3783 W	131	Crops and Grassland	25-Jul-14
Sheepdrove	SHEEP	51.530 N	1.482 W	170	Grassland	24-Oct-13
Sourhope	SOURH	55.480 N	2.230 W	487	Coarse Grassland	9-Dec-14
Spen Farm	SPENF	53.869 N	1.319 W	57	Arable and horticulture	23-Nov-16
Stoughton	STGHT	52.602 N	1.047 W	130	Arable	18-Aug-15
Stiperstones	STIPS	52.581 N	2.945 W	432	Heathland	6-Nov-14
Tadham Moor	TADHM	51.208 N	2.829 W	7	Grassland	14-Oct-14
Waddesdon	WADDN	51.840 N	0.948 W	98	Grassland	4-Nov-13



(a)



(b)



(c)

Fig. A1. Box plots of the statistical scores for comparison of absolute soil moisture for temporal collocated observations at 38 COSMOS-UK stations: (a) R ; (b) Bias; (c) ubRMSE.

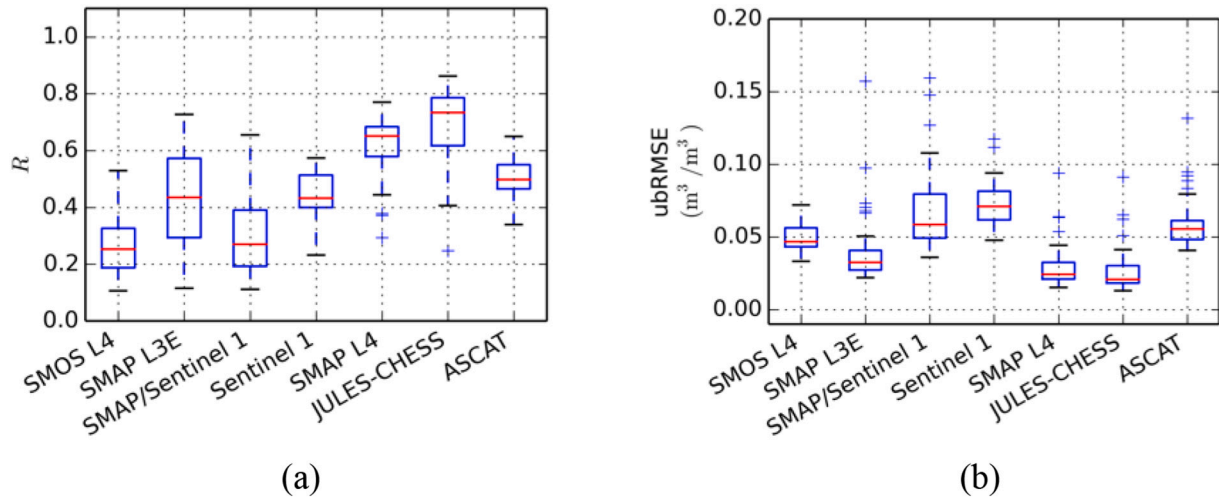


Fig. A2. Box plots of the statistical scores for comparison of soil moisture anomalies for temporal collocated observations at 38 COSMOS-UK stations: (a) R ; (b) $ubRMSE$.

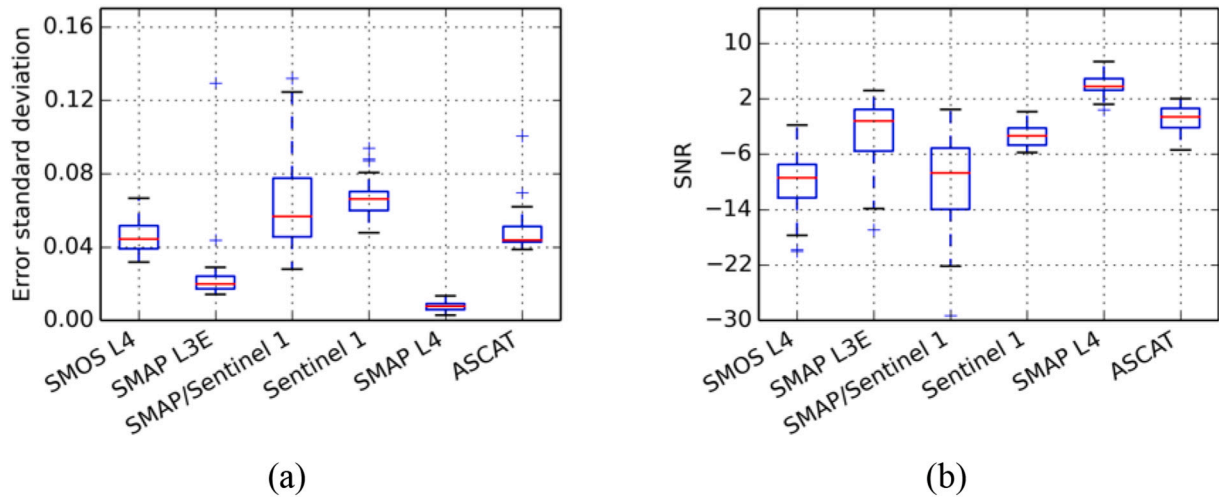


Fig. A3. Box plots of (a) the absolute error standard deviation, and (b) SNR [dB] for each satellite-based product calculated from the triple collocation analysis of soil moisture anomalies at all COSMOS sites.

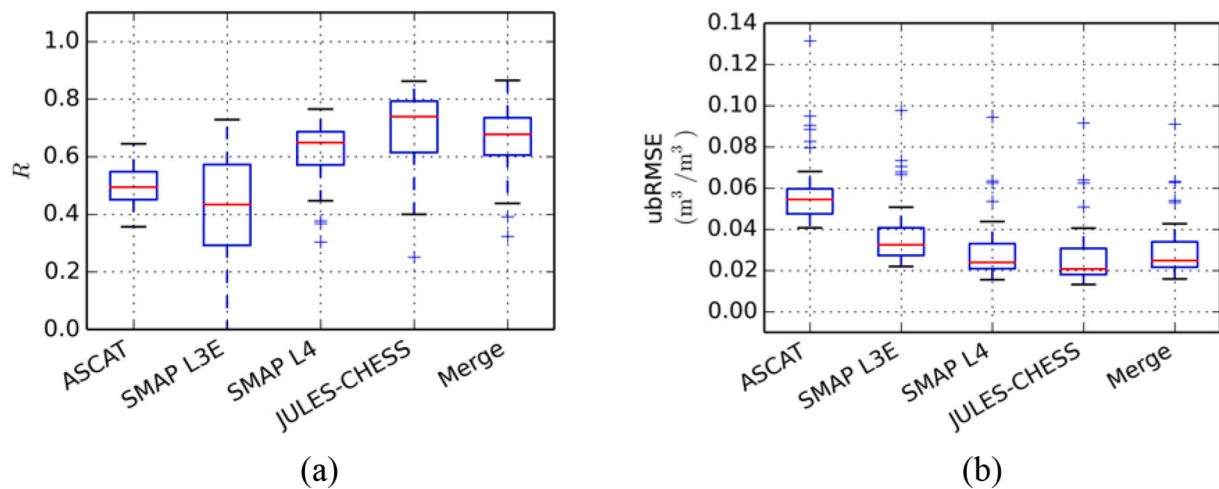


Fig. A4. Evaluation of SMOS L4, SMAP L3E, SMAP L4, JULES-CHESS, and merged soil moisture anomalies against COSMOS-UK measurements.

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