ESA Climate Change Initiative Plus - Soil Moisture

Product Validation and Intercomparison Report (PVIR)

Supporting Product version v09.1

Deliverable ID: D4.1 Version 2

20/06/2024

Submitted by

EODC Earth Observation Data Centre for Water Resources Monitoring GmbH

in cooperation with

TU Wien, VanderSat, ETH Zürich, CESBIO and INRAE

This document forms the deliverable D4.1 Version 2, Product Validation and Intercomparison Report (PVIR) and was compiled for the ESA CCI+ PHASE 2 - NEW R&D ON CCI ECVS Soil Moisture Project (ESRIN Contract No. 4000126684/19/I-NB).

For more information on the CCI programme of the ESA see https://climate.esa.int/en/.

Number of pages: 45 (including cover and preface)

Authors:	M. Hirschi, P. Stradiotti, W. Preimesberger, W. Dorigo, R. Kidd
Circulation (internal):	Project consortium and science partners
External:	ESA

Issue	Date	Details	Editor
0.1	19/04/2024	Document started based on deliverable D4.1, PVIR Version 1 of ESA CCI+ PHASE 2 - NEW R&D ON CCI ECVS Soil Moisture Project (issue 1.0, 01-08-2023, RD-01). Update of all analyses and figures and corresponding text with product version v09.1.	M. Hirschi, P. Stradiotti
0.2	19/06/2024	Inclusion of gap-filled v09.1 in the trends section	M. Hirschi
0.3	20/09/2024	Revised description of Figure 1. To ESA for approval.	M. Hirschi, P. Stradiotti, R Kidd
1.0	20/09/2024	Finalised	R. Kidd

For any clarifications, please contact Martin Hirschi (martin.hirschi@env.ethz.ch).

Project Partners	
Prime Contractor, Project Management	**EODC**, Earth Observation Data Centre for Water Resources Monitoring (Austria)
Earth Observation Partners	**TU Wien**, Vienna University of Technology (Austria)
	VDS, Vandersat (The Netherlands)
	CESBIO, CESBIO (France)
	INRAE, Institut National de la Recherche Agronomique (France)
Climate Research Partner	**ETH Zürich**, Institute for Atmospheric and Climate Science, (Switzerland)

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Acronyms

ABS	Absolute values of soil moisture
AMSR-E	Advanced Microwave Scanning Radiometer - Earth Observing System
ASCAT	Advanced SCATterometer
ATBD	Algorithm Theoretical Basis Document
CAL-VAL	Calibration and validation
CDF	Cumulative Distribution Function
CCI	Climate Change Initiative
CRDP	Climate Research Data Package
ECMWF	European Centre for Medium Range Weather Forecasts
ECV	Essential Climate Variable
ESA CCI SM	Soil moisture time series developed in the framework of ESA CCI
EO	Earth Observation
ERA	ECMWF Re-Analysis
ESA	European Space Agency
FY3	FengYun-3 satellites
IAA	Inter-annual anomalies of soil moisture
ISMN	International soil moisture network
LSM	Land surface model
MERRA-2	Modern-Era Retrospective analysis for Research and Applications, Version 2
NASA	National Aeronautics and Space Administration
NCAR	National Center for Atmospheric Research
NH	Northern Hemisphere
PUG	Product User Guide
PVIR	Product Validation and Intercomparison Report
PVP	Product Validation Plan
RMSD	Root mean square difference
RMSE	Root mean square error
SAC-SMA	Sacramento Soil Moisture Accounting model
SM	Soil moisture
SMAP	Soil Moisture Active Passive mission
SMOS	Soil Moisture and Ocean Salinity mission
SSM	Surface soil moisture
TUW	Vienna University of Technology
ubRMSD	Unbiased root mean square difference
VWC	Volumetric water content
WMO	World Meteorological Office

1 Executive Summary

Within the framework of the European Space Agency (ESA) Climate Change Initiative (CCI) soil moisture project, an over 40-year (1978-2023) soil moisture time series (ESA CCI SM v09.1) is developed, which consists of three products: an ACTIVE data set, a PASSIVE data set and a COMBINED data set. It provides daily surface soil moisture with a spatial resolution of 0.25°. The merged product as well as its active and passive sources are publicly available to the user on the project webpage (https://climate.esa.int/en/projects/soil-moisture/data/) and also from the CCI Open Data Portal (https://climate.esa.int/en/odp/#/dashboard). Furthermore, the detailed description of its development [ATBD, RD-02], and a product user guide [PUG, RD-03] are publicly available on the project webpage (https://climate.esa.int/en/projects/soil-moisture/key-documents/).

The validation of the public release of ESA CCI SM v09.1 is an important mechanism within the production process and is documented in this Product Validation and Intercomparison Report (PVIR). The guideline of the ESA CCI SM product validation is described in the Product Validation Plan [PVP, RD-05] and ensures that the validation meets the overall user requirements and that it is carried out in a transparent way. The established validation protocol is broadly accepted by the international soil moisture community. The validation is performed with in-situ or other appropriate global datasets (e.g., land surface models, land data assimilation systems, land reanalyses) that were not used for the production of the ESA CCI SM product. Additionally, the ESA CCI SM product releases undergo a basic “verification” as part of the production process, which is also documented in this PVIR.

The PVIR encompasses the following analyses (carried out independently by the indicated partners).

TU Wien: During the development of the ESA CCI SM product, verification and accuracy checks are undertaken to ensure that the product is made correctly and that the scientific developments implemented are positively impacting the product. The final results of these verification and accuracy checks are presented in this document (Section 5.1).

The verification checks include checking for completeness, i.e., spatial and temporal coverage for the new product and also with respect to the previous, approved (public), version of the product. These checks include ensuring the uncertainty data is provided with the product.

Basic validation is undertaken with respect to soil moisture from ECMWF’s 5th generation atmospheric reanalyses of the global climate (ERA5) to benchmark the product in space (spatial Pearson’s correlation) and to verify whether it is consistent with its previous version. For inter-comparison between versions, only the common observations are used.

The evaluation of ESA CCI SM v09.1 shows a slightly decreased spatial and temporal coverage and a stable validation performance compared to the last public version. The break-adjusting routine is now included in all distributed products.

ETH Zürich: After Verification, the ESA CCI SM product is validated over four regions (North America, Europe, Sub-Saharan Africa, and Australia) and globally using in-situ observations from the ISMN and using the ERA5-Land soil moisture reanalyses at 0.25° resolution (Section 5.2). In this validation process, the current release v09.1 is also set into perspective to previous major post-v3 releases of ESA CCI SM from v4.7 up to v08.1. The evaluation uses the two top layers of the ERA5-land soil moisture reanalyses (i.e., 0-7 cm and 7-28 cm depths) to compare the ESA CCI SM products, and the in-situ observations in 5 and 10 cm depth. In addition, the MERRA-2 reanalysis and GLDAS-Noah land-surface model, as well as an additional gap-filled version of the v09.1 COMBINED product is used in the analysis of the long-term temporal trends.

The evaluation shows no clear regions where the ESA CCI SM products agree very well or very poorly with in-situ observations. However, the highest and most consistent correlations were found over Australia where the in-situ observations were located in the same climatic region. The ESA CCI SM products correlate higher with the observed in-situ soil moisture at 5 cm than at 10 cm depth. This depth dependency was less clear for the comparison with ERA5-Land. Over the US, the ESA CCI SM products show higher correlation with the in-situ observations in areas of grassland than compared to areas of forest vegetation cover. This distinction for different vegetation types is less pronounced for the comparison with the ERA5-Land reanalysis.

Overall, the ESA CCI SM product releases show increasing correlations with in-situ data with the evolution of the product pointing to the mature state of the product (in particular visible for the more recent periods). The latest v08.1 and v09.1 show stable skill compared to the in-situ data.

However, large uncertainties remain in the representation of long-term temporal trends, which display distinct and partly diverging patterns among the ESA CCI SM COMBINED releases and the underlying ACTIVE and PASSIVE products, as well as compared to reanalysis and land-surface model products (Section 5.3).

2 Documents

2.1 Applicable documents

The documents outlined below detail the scope and focus for the work reported in this document.

[AD-1] ESA CCI+ PHASE 2 - NEW R&D ON CCI ECVS Soil Moisture Project Contract No: 4000126684/19/I-NB (CCN3).

[AD-2] Climate Change Initiative Extension (CCI+) Phase 2 New R&D on CCI ECVs, Statement of Work, ESA Earth Observation Directorate, ESA-EOP-SC-AMT-2021-56.

2.2 Reference documents

This section provides a list of reference documents either on which we base this document, or to which this document refers.

[RD-01] Product Validation and Intercomparison Report (PVIR), version 1, issue 1.0, 2023

[RD-02] Algorithm Theoretical Basis Document (ATBD), v9.1, 2024

[RD-03] Soil Moisture CCI Product User Guide (PUG), v9.1, 2024

[RD-04] Climate Research Data Package (CRDP), v9.1, 2024

[RD-05] Product Validation Plan (PVP), version 2, issue 1, 2024

2.3 Bibliography

A complete bibliographic list, detailing scientific texts or publications that support arguments or statements made in this document is provided in Section 7.

3 Introduction

3.1 Purpose of the document

The purpose of the PVIR is the final validation of the soil moisture time series, which is developed in the framework of the ESA CCI soil moisture project. It includes the verification and the validation of the product as outlined in the PVP.

3.2 Target audience

This document targets users of the soil moisture time series produced, as well as the scientific community. It demonstrates the value of an intercomparison between the ESA CCI SM product and other available soil moisture products.

3.3 Important documents

Detailed information on the ESA CCI SM v09.1 time series is provided in the Algorithm Development Document (ATBD, [RD-02]), as well as the Product User Guide (PUG, [RD-03]), produced in the framework of the ESA CCI soil moisture project. These documents are listed in Section 2 and are publicly available on the project webpage (https://climate.esa.int/en/projects/soil-moisture/key-documents/), and also from the CCI Open Data Portal (https://climate.esa.int/en/odp/#/dashboard).

4 Datasets overview

ESA CCI SM v09.1 validated in this PVIR covers the 1978-2023 time period in case of the COMBINED and the PASSIVE products, respectively the 1991-2023 time period in case of the ACTIVE product. It provides daily estimates of global surface soil moisture (i.e., top ~2-5 cm of the soil) at 0.25° spatial resolution. Data coverage is limited in the early years of the COMBINED product when only passive sensors are available. Microwave retrievals are impossible under snow and ice or when the soil is frozen, and complex topography, surface water, and urban structures have negative impacts on the retrieval quality [*Dorigo et al.*, 2017]. In addition, dense vegetation attenuates the microwave emission and backscatter from the soil surface and may mask the soil moisture signal. These limitations result in spatio-temporal data gaps of the product.

In ESA CCI SMv07.1, a flag for barren ground conditions has been included in the PASSIVE and COMBINED product as optional, meaning that soil moisture has not been masked where the flag is raised. In v08.1 version, the flagging strategy for barren ground was changed to a majority filtering, meaning that the flag is only raised when at least 50% of the observing sensors + 1 agree on the occurrence of barren ground. For a fair comparison of the latest two versions (v08.1 and v09.1) with the previous versions of the products, the flag is never applied in the analysis presented here. In addition, a break-adjustment in the COMBINED product is performed as of v08.1 using the methodology set out in *Preimesberger et al.* [2021; also described briefly in the ATBD [RD-02]]. For further details on the single ESA CCI SM product versions, please refer to the respective CRDP [RD-04].

The following table shows an overview of the datasets used for the validation of the ESA CCI SM product. Further details on these comparison datasets and the applied processing can be found in the respective parts of Sections 5.1 to 5.3.

Table 1: Overview of the products used for the ESA CCI SM validation.

Product	Producer	Data class	Description	Max. period used	Coverage
ISMN	Individual soil moisture networks, hosted at TU Wien	In-situ	In-situ soil moisture measurements	1991-2023	Global (but only few data in South America, Africa, and Asia)
ERA5-Land	ECMWF	Land surface model reanalysis	Reanalysis data for volumetric soil water at different levels of the soil profile	1988-2022	Global
ERA5	ECMWF	Atmospheric reanalysis	Reanalysis data for volumetric soil water at different levels of the soil profile	2007-2022	Global
MERRA-2	NASA	Atmospheric reanalysis	Reanalysis data for volumetric soil water at different levels of the soil profile	1988-2022	Global
GLDAS-Noah	NASA	Offline land surface model	Land-surface model data for different levels of the soil profile	2000-2022	Global

5 Verification and validation results

The following sections present the verification and validation results of the ESA CCI SM v09.1 product.

5.1 Verification and basic validation of the product

As part of the product generation, verification and basic validation activities are carried out throughout the development cycle and on the final product. The final generated dataset is evaluated here for completeness and to ensure the final products provide temporal and spatial patterns expected for soil moisture, through analysis of data statistics and soil moisture anomalies. The dataset is also compared to ERA5 to evaluate the physical plausibility of the ESA CCI SM products.

5.1.1 Datasets

ESA CCI SM

In addition to the newly generated datasets of ESA CCI SM v09.1, the previous public release (v08.1) and the anomalies for 2023 from the v202212 version of the Copernicus Climate Change Service[1] (C3S), based on v05.2, have been used[2]. All three respective products of ESA CCI SM (ACTIVE, PASSIVE, COMBINED) have been analysed, however, only a subset of these results is presented here. Further information is available upon request.

ERA5 soil moisture

ERA5 is a global reanalysis product provided by ECMWF [*Hersbach et al.*, 2020]. It provides global, sub-daily simulations of variables for land, atmosphere and ocean waves. The downloaded original 6-hourly (starting at 0:00 UTC) images of ERA5 Volumetric Soil Moisture and Soil Temperature with a spatial resolution of 0.25° Lat. x 0.25° Lon have been converted into a time series format of daily averages. The ERA5 dataset starts in 1979, however, in this comparison, a validation period of 2007-01-01 until 20221-12-31 is used.

5.1.2 Dataset completeness

The data coverage is as expected, with greater fractional coverage in the later periods and seasonally varying coverage at extreme latitudes due to snow cover (Figure 1). In addition, around the equator, coverage is reduced due to high vegetation cover in many areas where soil moisture cannot be reliably retrieved. At several points in time, step changes in the

[1] https://cds.climate.copernicus.eu/portfolio/dataset/satellite-soil-moisture
[2] Note that the v06.1 dataset runs to 2020-12-31 and therefore, comparisons to this dataset and the statistics presented here only use data up until that date with the exception of the Hovmöeller diagrams.

number of observations correspond to the start of specific missions (e.g., the start of the AMSR-E mission as of June 2006 is visible in both the PASSIVE and COMBINED products). These comments are applicable to all data products (COMBINED, PASSIVE and ACTIVE; Figure 1, Figure 5 and Figure 6 respectively).

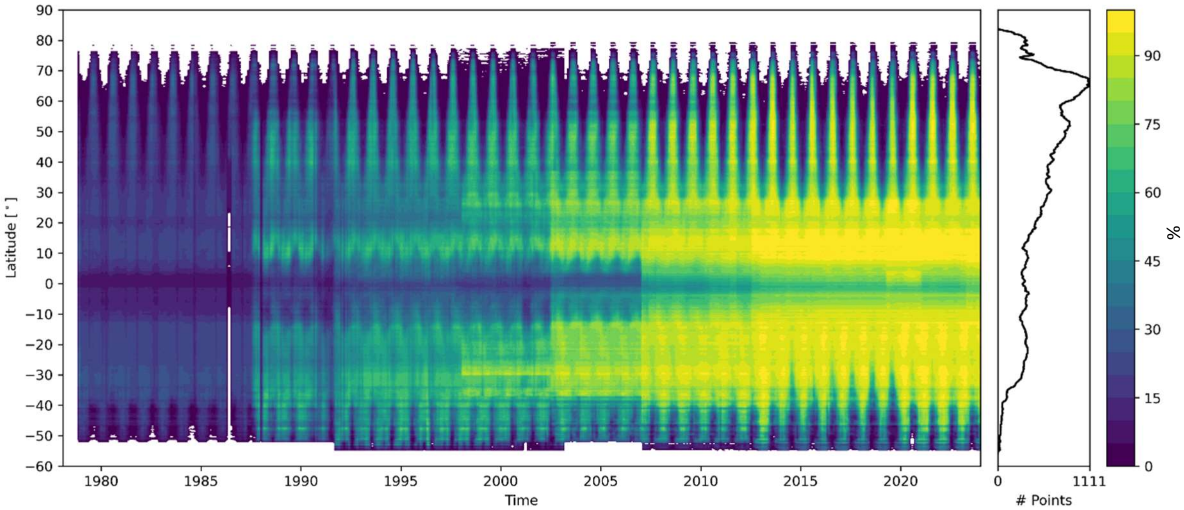

Figure 1: Hovmöller diagram of the fractional number of valid observations per month in the Soil Moisture variable of ESA CCI SM v09.1 COMBINED product (left) corresponding number of land points in the grid per latitude (right). Note: areas of mean C-Band VOD >.526 are masked out from the monthly / latitude aggregation.

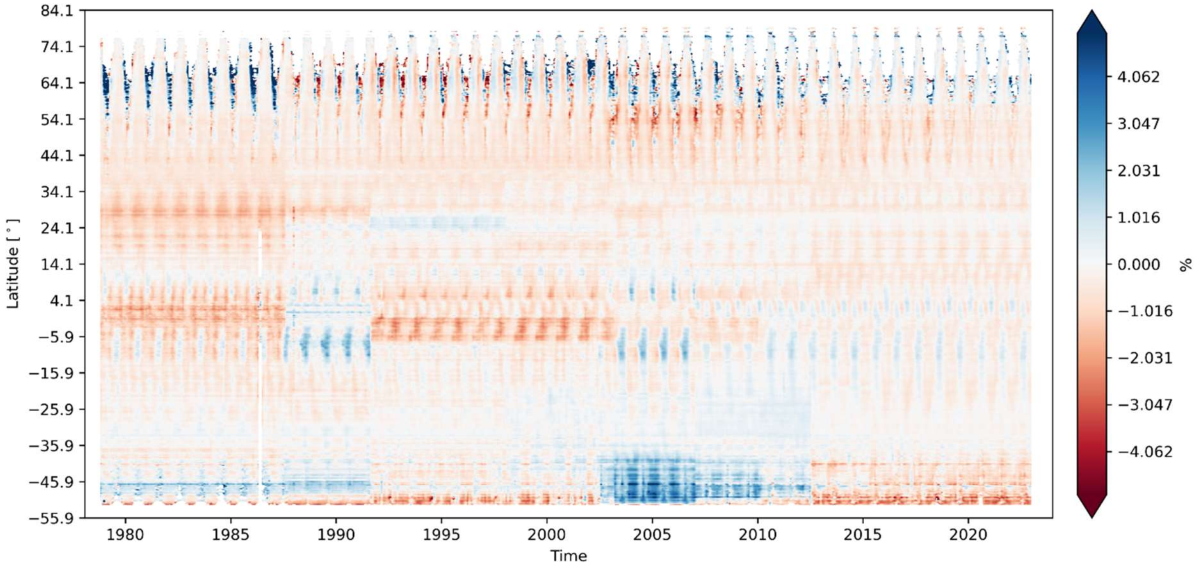

Figure 2: Hovmöller diagram of the difference in the fractional number of valid observations per month in the Soil Moisture variable of ESA CCI SM v09.1 COMBINED product compared to the ESA CCI SM v08.1 COMBINED product. Note: areas of mean C-Band VOD >.526 are masked out from the monthly / latitude aggregation.

In terms of the difference to the previous product (Figure 2), the fractional coverage has generally decreased (in the order of 1%), with localised gains relative to a specific sensor period and region (e.g., 2002-2012, -36° -56°). Such differences originate from changes in the merging methodology (most likely in the scaling step), rather than in the input data.

The spatial distribution of the coverage is provided in Figure 3 for the period 2007-01-01 to 2023-12-31 (i.e., post the introduction of soil moisture data from ASCAT sensors). As expected, there are fewer observations available in areas flagged for snow and vegetation cover. Although the observations flagged for barren grounds are included in the analysis, the coverage decreases naturally in desert and very dry areas for instance due to low weights obtained in the merging. This effect is also traceable to the impact of sub-surface scatter in barren soils.

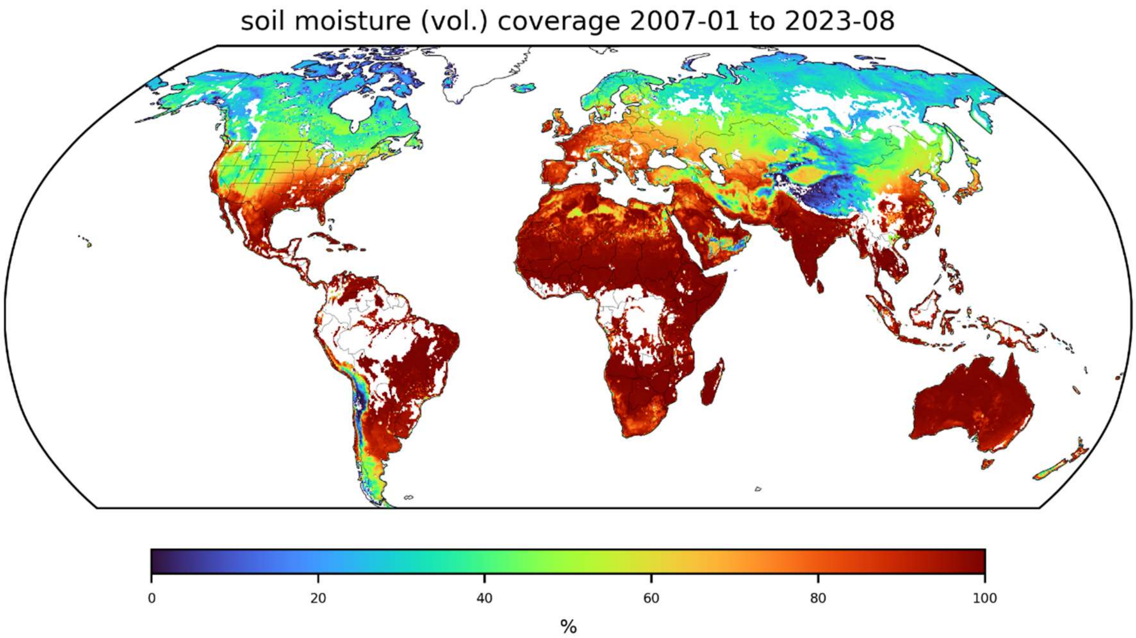

Figure 3: Spatial fraction of valid observations in the Soil Moisture variable of ESA CCI SM v09.1 COMBINED product for the period 2007-01-01 to 2023-12-31. Note: areas of mean C-Band VOD >.526 are masked out.

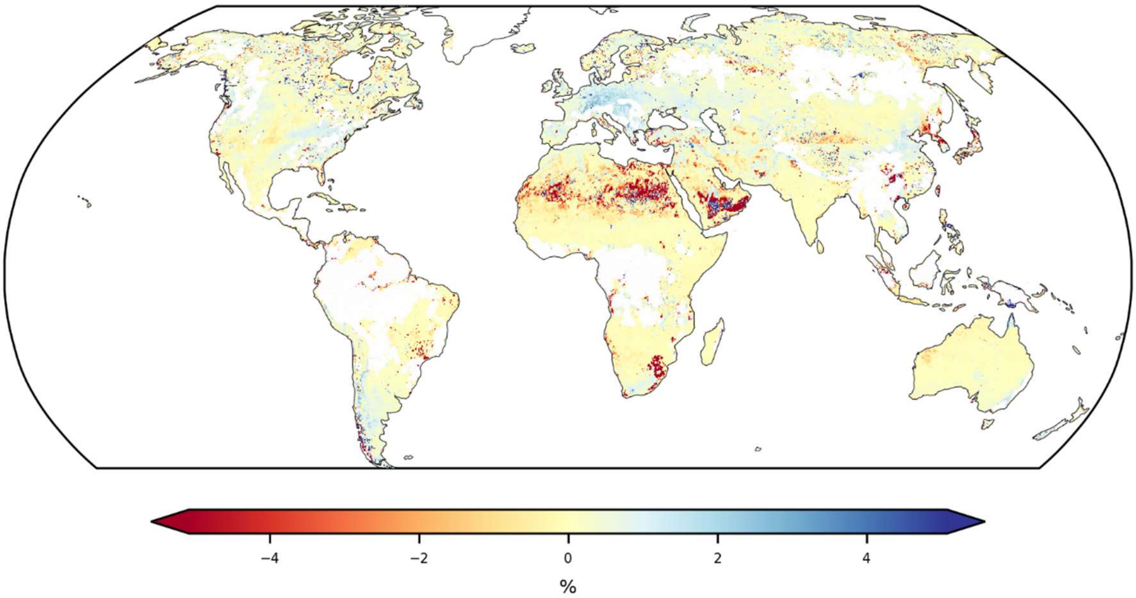

Figure 4: Difference in the spatial fraction of valid observations in the Soil Moisture variable of ESA CCI SM v09.1 COMBINED and v08.1 for the period 2007-01-01 to 2022-12-31. Blue represents an increase in coverage in the new (v09.1) product. Note: areas of mean C-Band VOD >.526 are masked out.

In spatial terms, the coverage has likewise remained homogeneous in the period after 2007 (Figure 4). A slight decrease in coverage is observable for a few areas in and around the Sahara desert region, in the Arabic peninsula, and in eastern South Africa, while a slight increase can be observed for central-eastern Europe, eastern US, and southern South America (Figure 4).

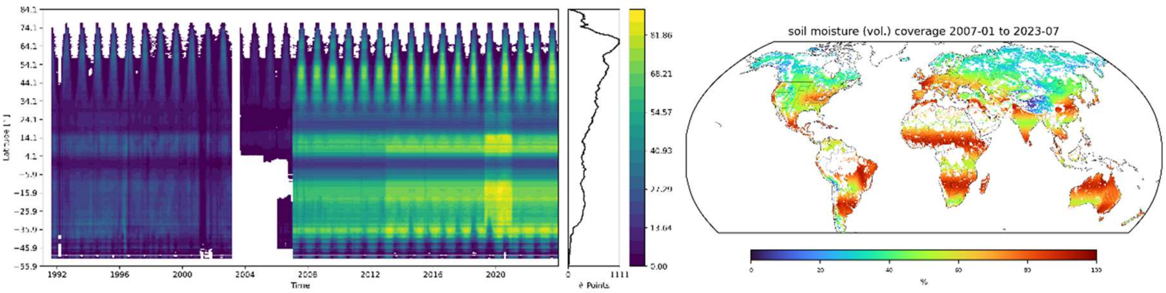

Figure 5: As Figure 1, but for the ESA CCI SM v09.1 ACTIVE product (left) with the spatial distribution of valid observations for the period 2007-01-01 to 2023-12-31 (right). Note: areas of mean C-Band VOD >.526 are masked out from the monthly / latitude aggregation.

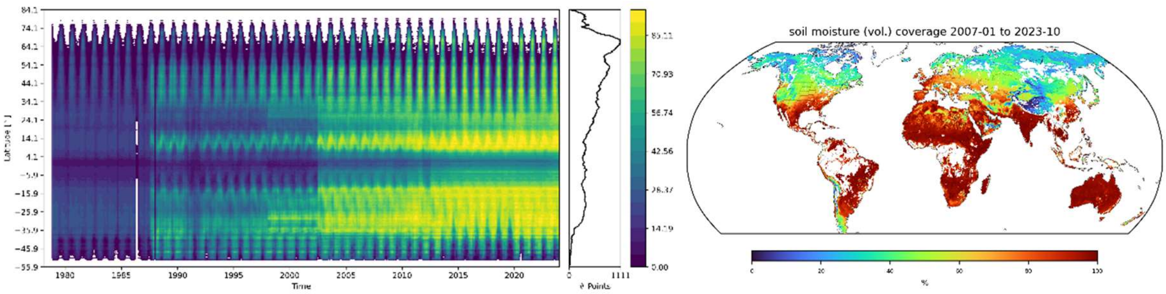

Figure 6: As Figure 1, but for the ESA CCI SM v09.1 PASSIVE product (left) with the spatial distribution of valid observations for the period 2007-01-01 to 2023-12-31 (right). Note: areas of mean C-Band VOD >.526 are masked out from the monthly / latitude aggregation.

5.1.3 Dataset uncertainty

Figure 7 shows changes in the uncertainty variable in ESA CCI SM v09.1 COMBINED over time / latitude. Uncertainty values are derived from the Triple Collocation (TC) process which can only be carried out when there are three independent soil moisture datasets available (an active, passive and modelled dataset are used in ESA CCI SM). For this reason, uncertainty values cannot be derived for SMMR and therefore, are only provided from the start of SSM/I (1987-07-09) onwards.

It can be seen from Figure 7 that the uncertainty reduces over time with the most recent periods showing uncertainty of below 0.01. This is due to the larger number of values from individual sensors used in the averaging and the optimality of the weighting. The uncertainty is also characteristic of the variability of soil moisture, with accuracy comparatively increasing in low-variability areas such as deserts (latitudes between 15° and 35° North). A seasonal pattern emerges due to the underlying seasonality of the environmental parameters that affect the retrieval. The pattern alternates between Hemispheres, following the growth of vegetation and its attenuation of the signal.

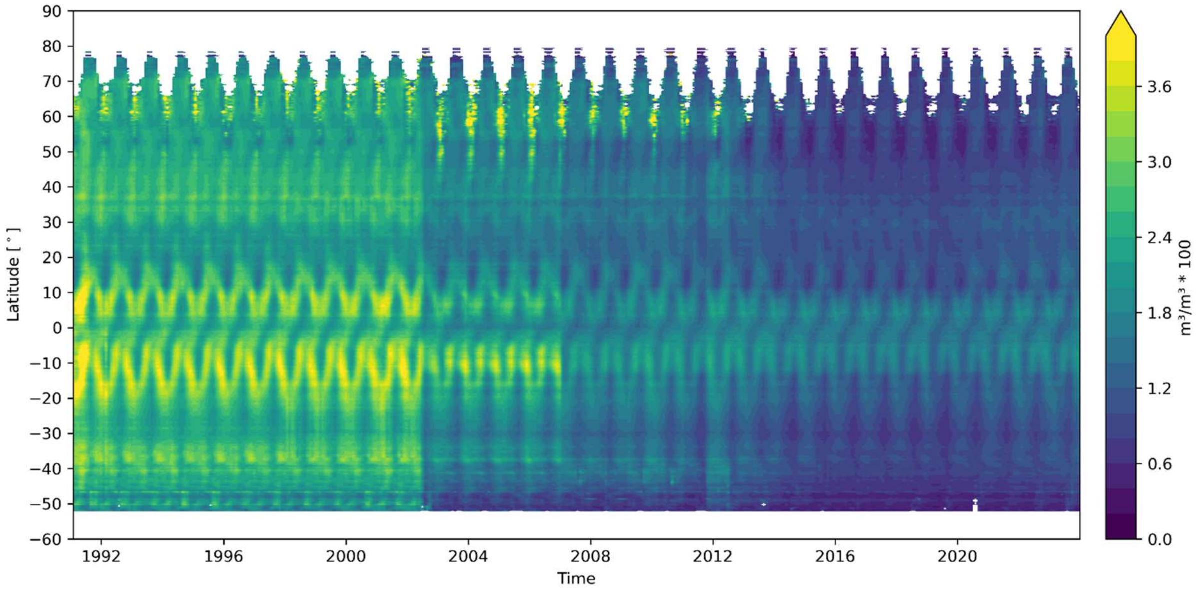

Figure 7: Monthly soil moisture uncertainty in ESA CCI SM v09.1 COMBINED. Note: areas of mean C-Band VOD >.526 are masked out from the monthly / latitude aggregation.

5.1.4 Soil moisture statistics

The mean and standard deviation of the ESA CCI SM v09.1v09.1 COMBINED product (Figure 8 and Figure 9) have been calculated for the period 2007-01-01 to 2023-12-31 and compared to the results from the v08.1 COMBINED product for the common period 2007-01-01 to 2021-12-31 (Figure 10).

The spatial patterns shown for both the mean and standard deviation are as expected, with regions of seasonal precipitation regimes showing high variability as opposed to low variability for instance in deserts and other arid areas. Looking at the comparison of the mean and standard deviation statistics on a per-point level, v09.1 remains consistent with the previous product version. The most noticeable differences are for low variability regimes (Figure 10, right) and only at specific locations (not shown).

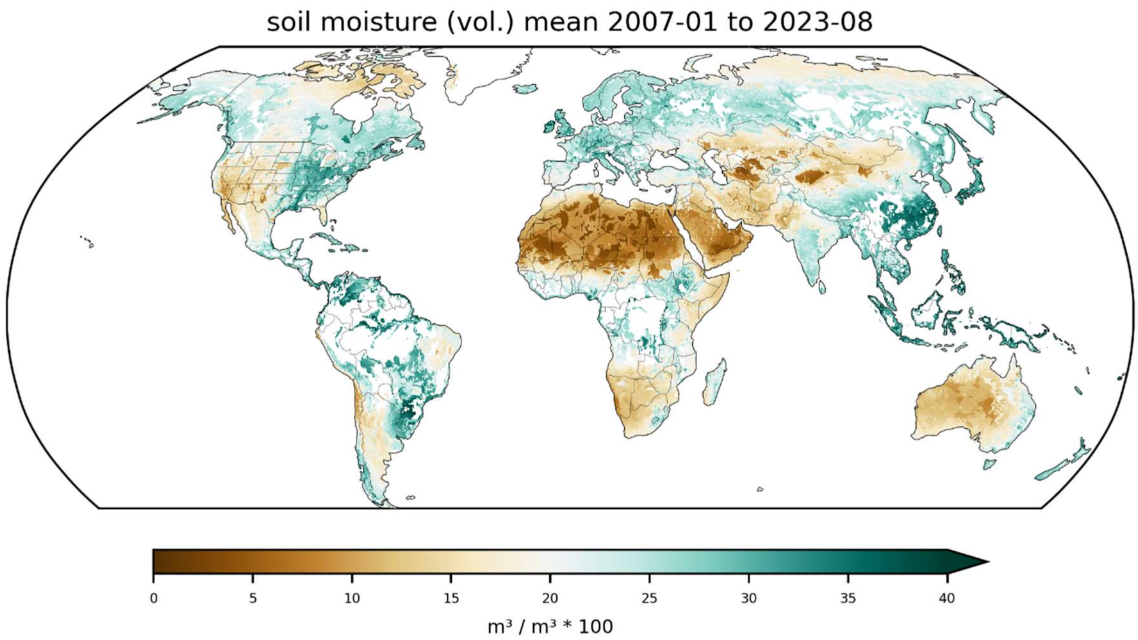

Figure 8: Mean soil moisture for the ESA CCI SM v09.1 COMBINED product for the period 2007-01-01 to 2023-12-31. Note: areas of mean C-Band VOD >.526 are masked out.

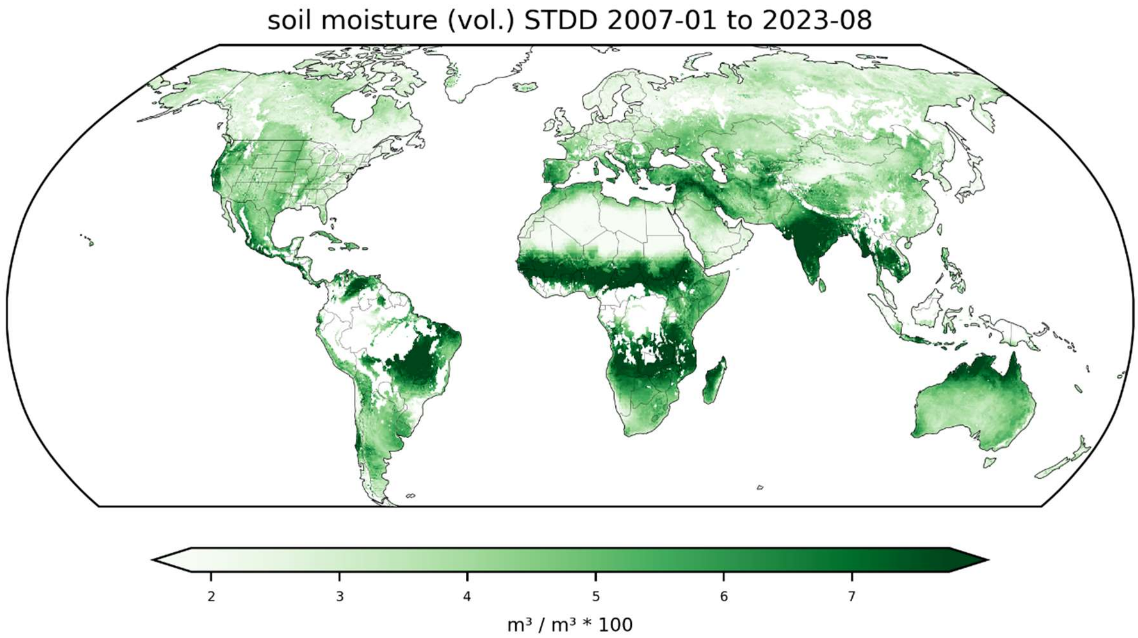

Figure 9: Standard deviation of soil moisture for the ESA CCI SM v09.1 COMBINED product for the period 2007-01-01 to 2023-12-31. Highlighted are the values below (red) and above (cyan) the 5th and 95th percentile, respectively. Note: areas of mean C-Band VOD >.526 are masked out.

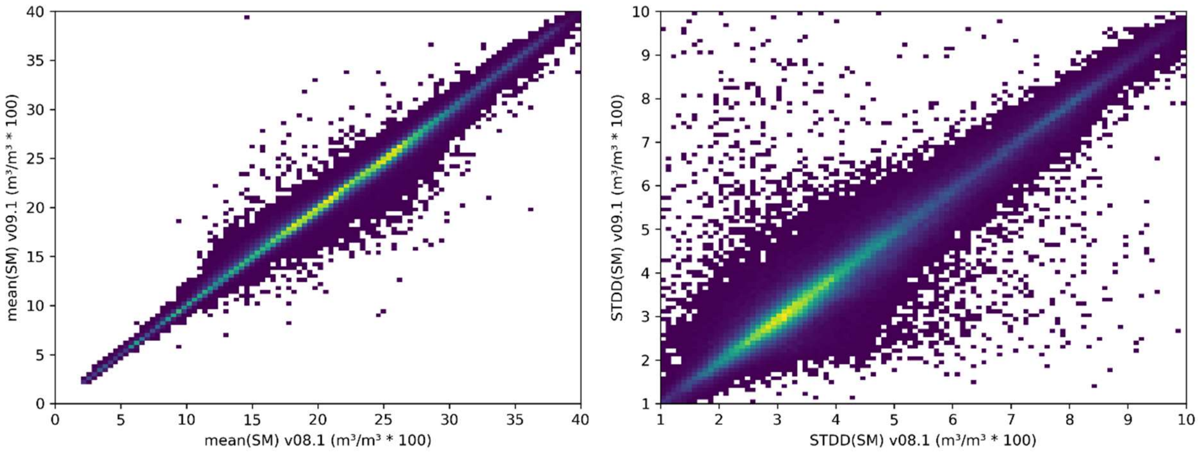

Figure 10: Comparison of the mean (left) and standard deviation (right) of the ESA CCI SM v09.1 and v08.1 COMBINED datasets. Relative to the period 2007-01-01 to 2022-12-31.

5.1.5 Soil moisture anomalies

Soil moisture anomalies are generated for each ESA CCI SM product version and used in the BAMS State of the Climate (SotC) report [e.g., *Preimesberger et al.*, 2020]. For the verification of the product, simple visual inspection of the anomalies provides a quick check of how the product is performing compared to previous products (i.e., do the anomalies provide the same spatial patterns) and can be easily verified using knowledge of the extreme drought and rainfall events in the period analyzed.

Figure 11 shows the anomalies for the year 2023 for Europe for the ESA CCI SM v09.1 COMBINED product. The same is shown in Figure 12 for the v202212 version of C3S Soil Moisture, which is based on an operational version of ESA CCI SM v05.2.

The patterns coincide well between the two product versions, with the anomalies of both reflecting the transition of ENSO from La Niña to El Niño conditions that occurred in 2023. Wet soil moisture conditions were recorded in northern Australia, in India, in parts of East Asia, as well as in parts of northeast Brazil and the Horn of Africa, while dry conditions occurred in the River Plate basin and Patagonia, and in the Canadian Prairies . Although the patterns coincide well, the magnitude of the anomalies is in general lower in the new v09.1 product. The same was noticed for the comparison of the previous ESA CCI SM version in the year 2022 [ATBD, RD-02] and is possibly caused by the lower number of sensor used in the C3S v202212 version, which leads to higher noise in the data. In general, no major discontinuities are found between the two versions, which suggest that the performance in the product releases has stabilized.

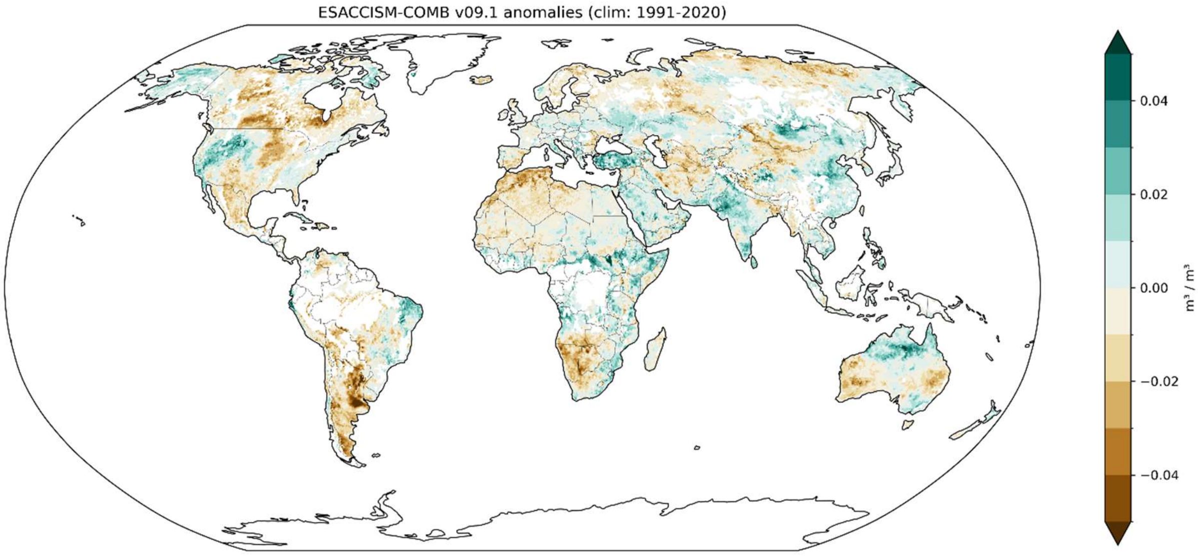

Figure 11: Soil moisture anomalies for the year 2023 from the ESA CCI SM v09.1 COMBINED product (reference period 1991-2020). Note: areas of high vegetation are masked out.

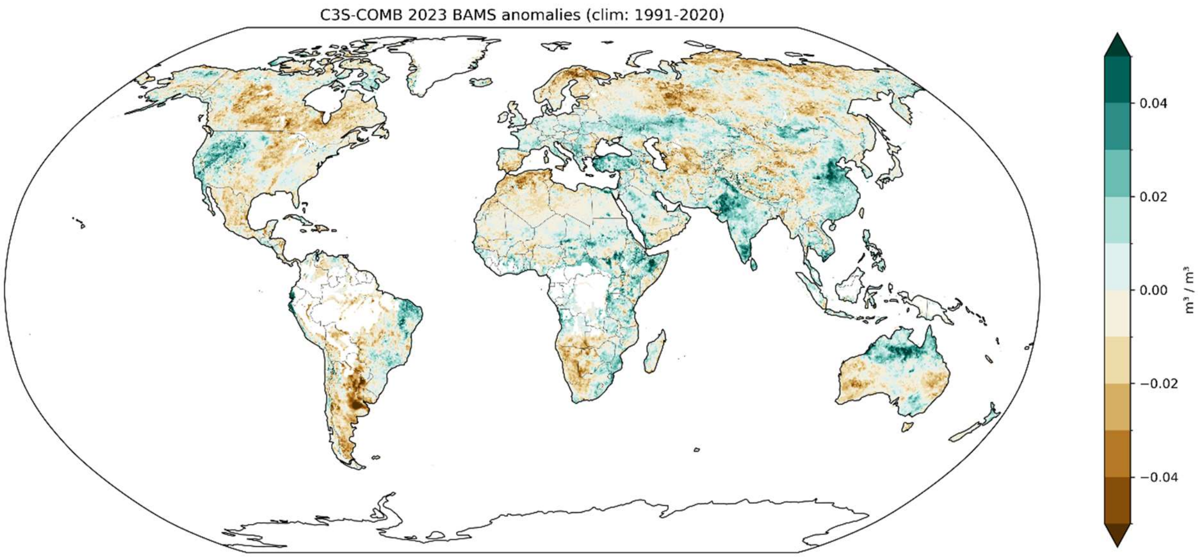

Figure 12: Soil moisture anomalies for the year 2023 from the C3S v202212 COMBINED product (reference period 1991-2020). Note: areas of high vegetation are masked out.

5.1.6 Basic validation against ERA5 soil moisture

Validation of ESA CCI SM v09.1 COMBINED against ERA5 soil moisture has been undertaken using the QA4SM framework (www.qa4sm.eu) run locally to allow the inclusion of v09.1. An inter-comparison (i.e., common observations only) was undertaken using v09.1 COMBINED, v08.1 COMBINED and ERA5 soil moisture for the period 2007-01-01 to 2022-12-31.

This period has been chosen as there are more observations available in this period (see Figure 1) and the majority of the changes made at v09.1 affect this period. This means that that the validation results provide clearer information about how the product has changed between v08.1 and v09.1.

No scaling has been undertaken between the datasets prior to validation (since they are all provided in volumetric units) and spatial matching is undertaken using nearest neighbor resampling (CCI is matched to the nearest ERA5 point and results are presented on the ERA5 grid). Temporal matching is also undertaken using nearest neighbor resampling (i.e., the ERA5 observation closest to the midnight UTC timestamp of CCI is used).

The correlation between ERA5 soil moisture and ESA CCI SM v09.1 COMBINED is shown in Figure 13. As expected, good correlations are achieved in areas where the landcover characteristics are more optimal for retrieval, for instance in the sparsely vegetated plains and croplands in the Midwestern United States. Processes that affect the observational quality, e.g., frozen or barren soils (note that the flag for barren grounds is not applied to the data set), are associated with areas of low correlation at northern latitudes or on deserts.

Figure 14 shows the difference in correlation with ERA5 between v09.1 and v08.1. The correlation with the model was in general slightly decreased (mean -0.0032 (+- 0.058 Std. dev.) (-)), with local degradations in eastern China, the subpolar region and particularly in North America, and the Sahara and Arabian peninsula deserts. Slight improvements are also visible over eastern Europe, central Asia, and Australia. Overall, the patterns of degradation are comparable with the window size prescription maps used in the scaling with the objective to avoid the superposition of GLDAS signal over the observations [RD-02].

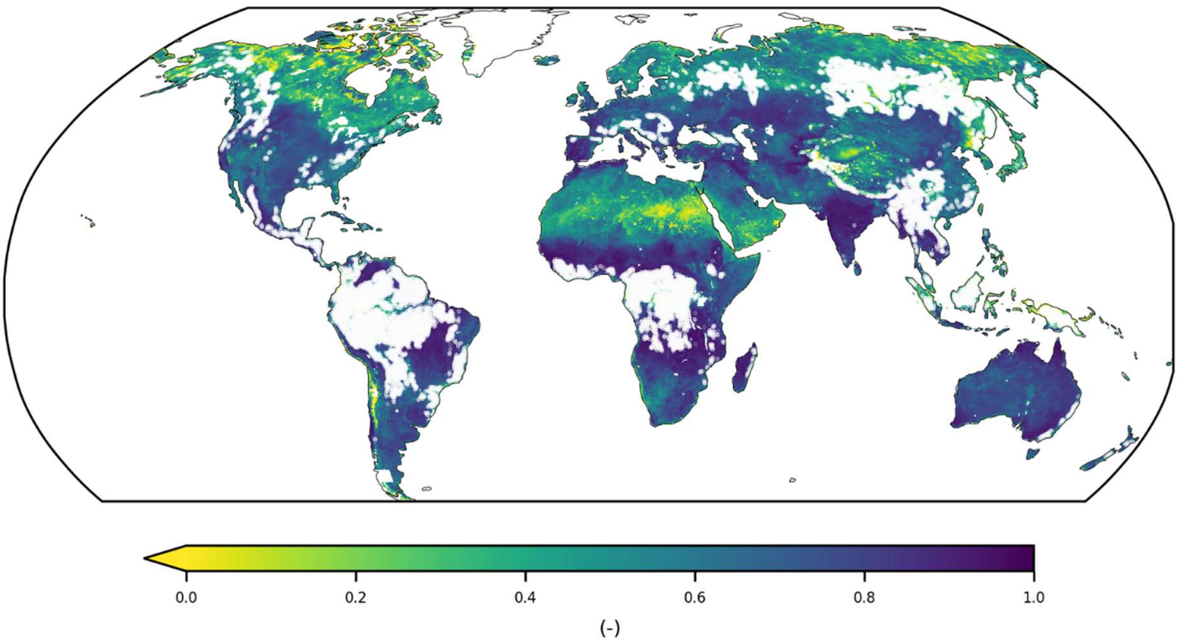

Figure 13: Pearson's correlation between ESA CCI SM v09.1 COMBINED and ERA5 soil moisture for the period 2007-01-01 to 2022-12-31. Note: areas of high vegetation are masked out.

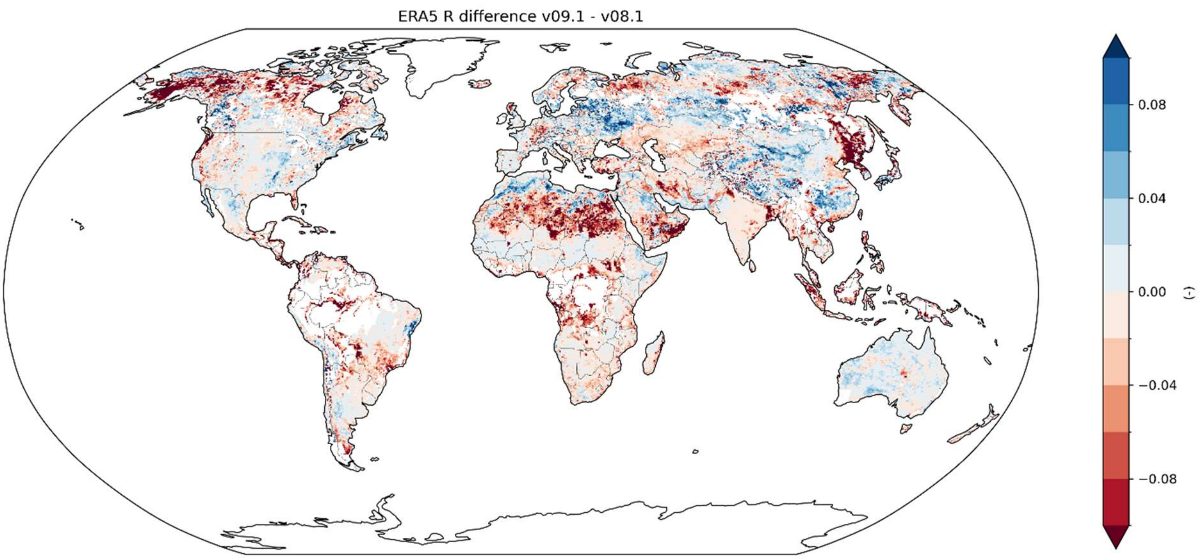

Figure 14: Difference in Pearson's correlation against ERA5 soil moisture between ESA CCI SM v09.1 COMBINED and v08.1 COMBINED for the period 2007-01-01 to 2022-12-31. Median diff (+- STD. Dev): -0.0032 (+- 0.058)

5.1.7 Summary

The following points summarize the conclusions of the above sections:

- The ESA CCI SM v09.1 product provides an overall stable coverage for COMBINED, ACTIVE, and PASSIVE compared to the previous version. A net albeit small (~1%) decrease in coverage is observed globally.
- The general statistics of the data are as expected, and in line with previous versions, with only local changes in SM standard deviation for low variability regimes.
- The soil moisture anomalies for 2022 in v09.1 COMBINED are in line with the previous v07.1 version (from v202212 of the operational C3S service), with patterns coinciding almost everywhere. The magnitude of the anomalies is generally lower compared to that found with the previous product version.
- The comparison with ERA5 in terms of correlation confirms the results obtained with previous product versions, and that the new v09.1 product remains stable (mean Pearson's R difference with v08.1: -0.0032 (-)).

5.2 Comparison to in-situ observations from ISMN and global land reanalysis products

5.2.1 Datasets and data processing

ESA CCI SM

To date various versions of the ESA CCI SM product are available. We use here v04.7, v05.2, v06.1, v7.1, v08.1 and the newest v09.1 release of the COMBINED product derived from the collocated C-band scatterometer data set and the collocated multi-frequency radiometer data set. These represent the major post-v3 releases of the different product generations [as represented by the evolution of the merging algorithm; see *Gruber et al.*, 2019 for an overview on the ESA CCI SM product evolution]. Additionally, the ACTIVE and PASSIVE products of ESA CCI SM v09.1 and v08.1 are used for some of the analyses. For the analysis of the long-term temporal trends, also an additional gap-filled version of the COMBINED product is considered, which is being produced as of v08.1 as a research product of ESA CCI SM [*Preimesberger et al.*, 2024]. The spatial resolution of ESA CCI SM is 0.25°, with daily temporal resolution. Data is presented in $m^3 m^{-3}$ and represents soil moisture in the top few millimeters to centimeters of the soil [*Kuria et al.*, 2007]. The quality and availability of the data has increased over time, as the number of available satellites has increased [*Dorigo et al.*, 2017; *Dorigo et al.*, 2015; *Dorigo et al.*, 2010].

ISMN

In-situ soil moisture measurements are obtained from the International Soil Moisture Network (ISMN). The ISMN database consists of measurements from various networks. If needed the data is transformed so that it is consistent in units ($m^3 m^{-3}$), then quality checked and flagged [*Dorigo et al.*, 2021; *Dorigo et al.*, 2011]. The analyses are based on a full download from 1 March 2024. All data is aggregated to daily averages, considering only values with quality flag "G" (see https://ismn.geo.tuwien.ac.at/en/data-access/quality-flags/). This implicitly also masks soil temperatures < 0°C.

Measurements from both the 5 cm and the 10 cm depths are considered since near-surface sensors appear to be more prone to errors [*Mittelbach et al.*, 2012].

ERA5-Land, MERRA-2, GLDAS-Noah

To determine the influence of soil depth on soil moisture variability, we use ECMWF's ERA5-Land reanalysis soil moisture [*C3S*, 2019; *Munoz-Sabater et al.*, 2021]. ERA5-Land is available as a re-gridded 0.25° soil moisture product, corresponding to the ESA CCI SM resolution, and has global coverage. Here we use the top two soil layers, which represent 0-7 cm and 7-28 cm soil depths. Data is aggregated from the original hourly temporal resolution to daily averages. For the analysis of the long-term temporal trends, also surface soil moisture of the atmospheric reanalysis MERRA-2 [*Gelaro et al.*, 2017] as well as GLDAS-Noah v2.1 ([*Rodell et al.*, 2004]) offline land surface model output is included.

Data selection

We consider ISMN soil moisture measurements that have at least one year of data (i.e., 365 days with valid data) and focus the main analyses on the US, Europe, Africa and Australia (see Figure 15) as well as the time period 1992-2019 when considering the major post-v3 ESA CCI SM product releases. This selection results in 1303 individual soil moisture time series from 44 different networks (see Figure 16). Soil moisture time series from the grid cells in which the stations fall are extracted from ESA CCI SM and ERA5-Land for this comparison. Thus, depending on the spatial and temporal overlap with ESA CCI SM, less time series might be used in the actual validation process.

Moreover, an extended time period is used for the global validation of the last two product releases (see Section 5.2.2) and the evaluation of the product evolution over time (see Section 5.2.3).

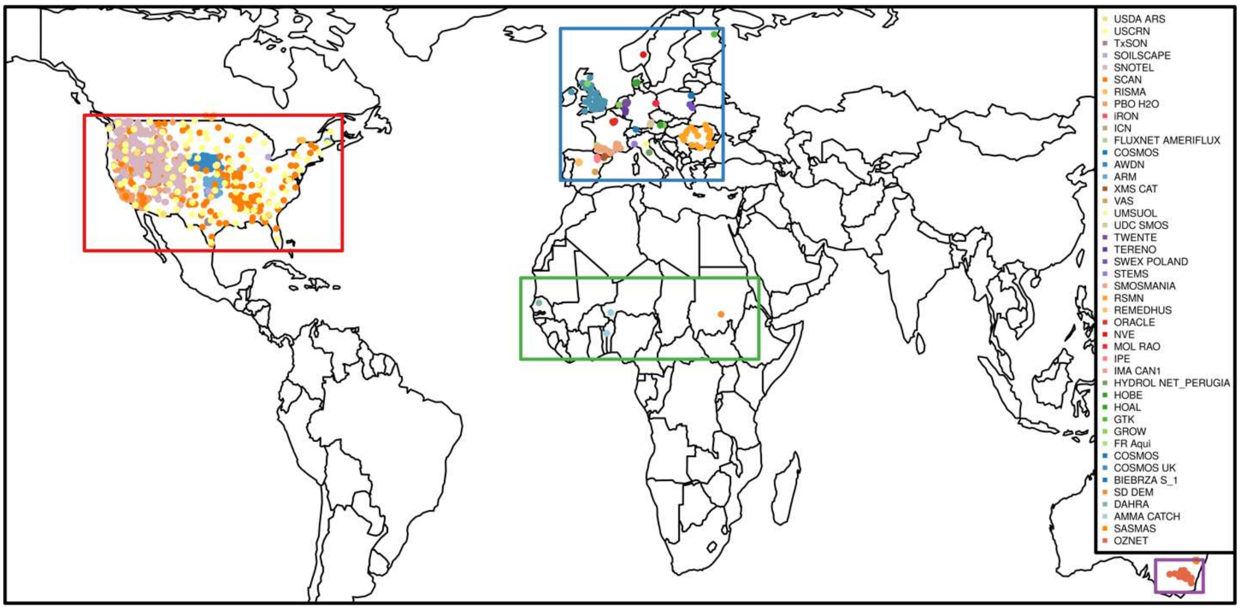

Figure 15: Overview of the spatial coverage of the stations considered in this section, rectangles indicate the four focus areas of the comparison, i.e., the United States (US, red), Europe (EU, blue), Africa (AF, green), and Australia (AUS, purple). Stations are color coded by network, see Figure 16 for the legend.

Comparisons of the products

We focus on the evaluation of ESA CCI SM v09.1 COMBINED and compare it to its forerunners v04.7, v05.2, v06.1, v7.1, v08.1 as well as to ERA5-Land layer 1 and layer 2 soil moisture. Additionally, the ACTIVE and PASSIVE products of v09.1 and v08.1 are used in some of the comparisons. All considered data sets have a different temporal coverage, and we account for this by masking for common data availability (unless specified otherwise; see Figure 16).

To account for the different units and dynamic ranges of the products, and to remove systematic differences between the products, the ESA CCI SM and ERA5-Land soil moisture time series are scaled to the respective in-situ time series using a CDF matching approach. Then, the long-term inter-annual anomalies are calculated based on subtracting the long-term mean using a 11-day window.

Agreement between in-situ data and ESA CCI SM and ERA5-Land is determined by the Pearson correlation and by the unbiased root mean square difference (ubRMSD) between the in-situ time series and the corresponding time series from the gridded product. Note that because data availability varies among locations, the time period (and amount of data) used to calculate the statistical metrics may differ between locations. Also, most of the available in-situ data is from the US, so a general global conclusion cannot be made. All analyses are performed on mean daily soil moisture, and results are shown for both the absolute scaled data, as well as the inter-annual anomalies.

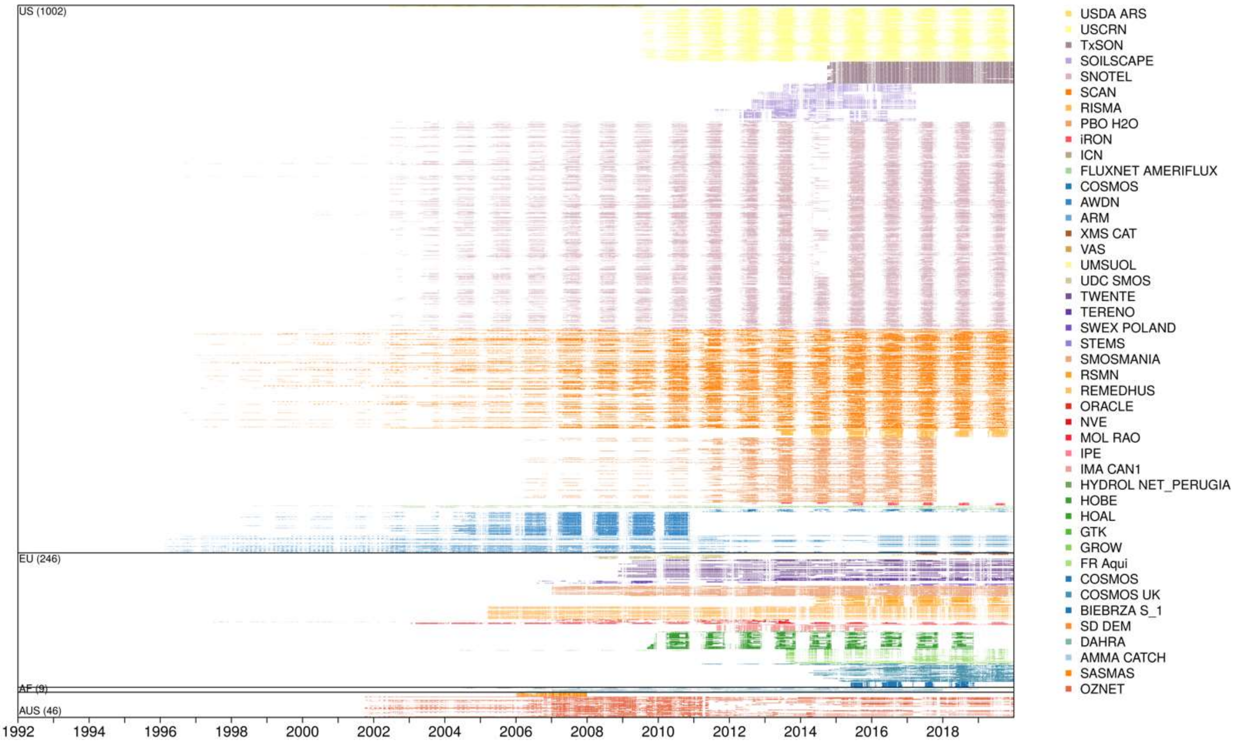

Figure 16: Overview of the temporal coverage of the stations considered in this section, after masking for common data availability, split per region. The number of stations per region is indicated in brackets.

5.2.2 General findings

Figure 17 shows the distribution of the correlation and ubRMSD values from the comparison of ESA CCI SM v08.1 and v09.1 (COMBINED, ACTIVE, PASSIVE) with respect to the full set of ISMN stations (i.e., about 1000 stations, 5 cm measuring depth) over the common 1992-2022 time period. Both absolute soil moisture values as well as the inter-annual anomalies are analyzed. The corresponding median values of the metrics and the corresponding confidence intervals are displayed in Table 2 and Table 3.

For the COMBINED product, similar correlations can be observed for v09.1 as compared to v08.1 with an (non-significant) decrease in the median correlation from 0.683 to 0.675 for the absolute soil moisture values and identical values of 0.536 for the inter-annual anomalies. The corresponding correlations for the ACTIVE and the PASSIVE product also remained constant between v08.1 and v09.1 (based on the confidence intervals of the median estimates, Table 2 and Table 3). The same holds for the ubRMSD, where v08.1 and v09.1 show very similar values. As expected, the PASSIVE and in particular the ACTIVE products show lower skill compared to the COMBINED products for both releases, showing the benefit of the applied merging approach for ESA CCI SM.

Overall, ERA5-Land shows better agreement with the in-situ data as compared to the ESA CCI SM releases, which is in line with other product inter-comparison studies [e.g., *Beck et al.*, 2021].

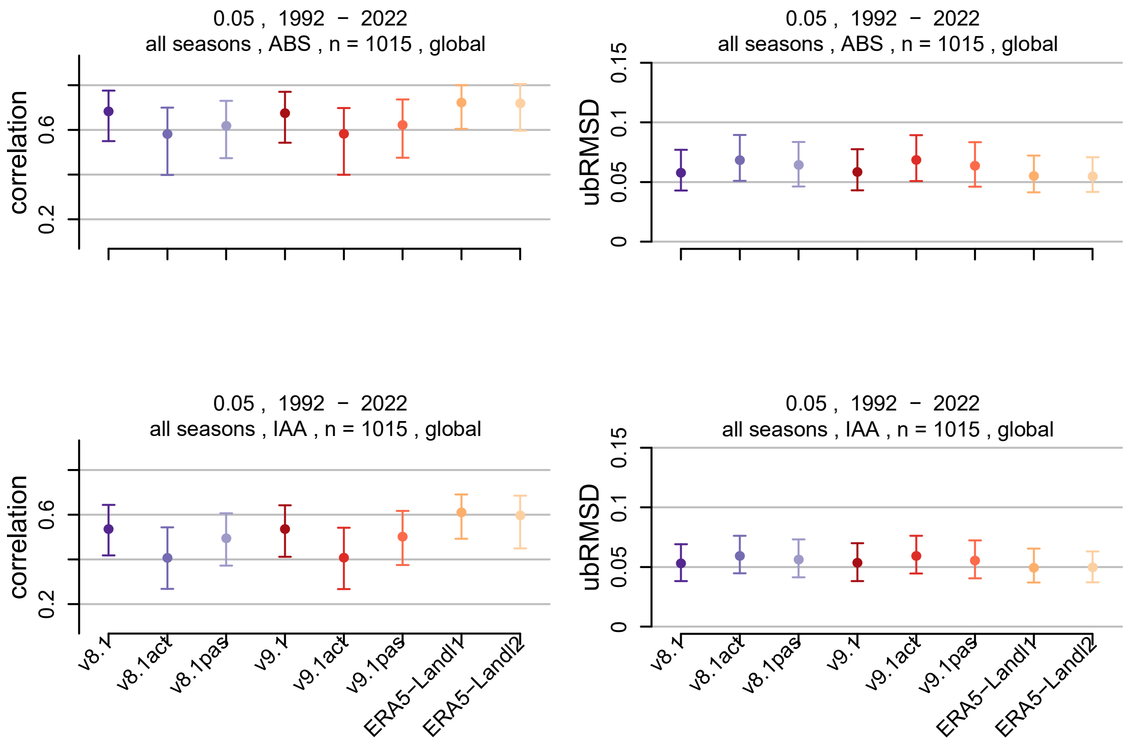

Figure 17: Correlation (left) and ubRMSD (right) of the last two releases of ESA CCI SM (v08.1 and v09.1 COMBINED, ACTIVE and PASSIVE; the latter two denoted as vX.Yact and vX.Ypas) as well as of ERA5-Land (layers 1 and 2)) as compared to the full set of ISMN in-situ station observations (5 cm measurement depth) for absolute soil moisture (ABS, top) and the inter-annual anomalies (IAA, bottom).

Table 2: Median (and corresponding 95% confidence intervals derived from a non-parametric bootstrap) of correlation and ubRMSD derived from the comparison ESA CCI SM v08.1 and v09.1 COMBINED, ACTIVE and PASSIVE to the full set of ISMN stations (measurements at 5 cm depth). Values are displayed for the absolute soil moisture.

Metric	COMBINED		ACTIVE		PASSIVE	
	v08.1	v09.1	v08.1	v09.1	v08.1	v09.1
Correlation [-]	0.683 [0.669;0.698]	0.675 [0.657;0.689]	0.582 [0.565;0.596]	0.582 [0.564;0.598]	0.618 [0.600;0.633]	0.622 [0.604;0.637]
ubRMSD [m³/m³]	0.058 [0.056;0.059]	0.059 [0.056;0.060]	0.069 [0.066;0.071]	0.069 [0.066;0.071]	0.064 [0.062;0.067]	0.064 [0.062;0.066]

Table 3: As Table 2 but for the inter-annual anomalies of soil moisture.

Metric	COMBINED		ACTIVE		PASSIVE	
	v08.1	v09.1	v08.1	v09.1	v08.1	v09.1
Correlation [-]	0.536 [0.520;0.546]	0.536 [0.524;0.549]	0.407 [0.388;0.420]	0.408 [0.392;0.421]	0.495 [0.484;0.509]	0.502 [0.493;0.517]
ubRMSD [m³/m³]	0.053 [0.052;0.055]	0.054 [0.052;0.056]	0.059 [0.058;0.062]	0.059 [0.057;0.062]	0.056 [0.054;0.058]	0.056 [0.053;0.057]

For different climate zones (Figure 18 and Figure 19), the correlations and ubRMSDs also often indicate better agreement of ERA5-Land with the in-situ data compared to different ESA CCI SM COMBINED releases, i.e., considering the major post-v3 releases of the main product generations [as represented by the evolution of the merging algorithm; see *Gruber et al.*, 2019]. In terms of correlations, the overall skill of ESA CCI SM tends to be slightly better for the temperate/continental summer dry climate zones (i.e., Csx/Dsx) for absolute values, but worse for the anomalies. A slight increasing tendency in the skill is visible for the subsequent major post-v3 ESA CCI SM releases. As above, PASSIVE and in particular the ACTIVE products of v09.1 show lower skill compared to the COMBINED products.

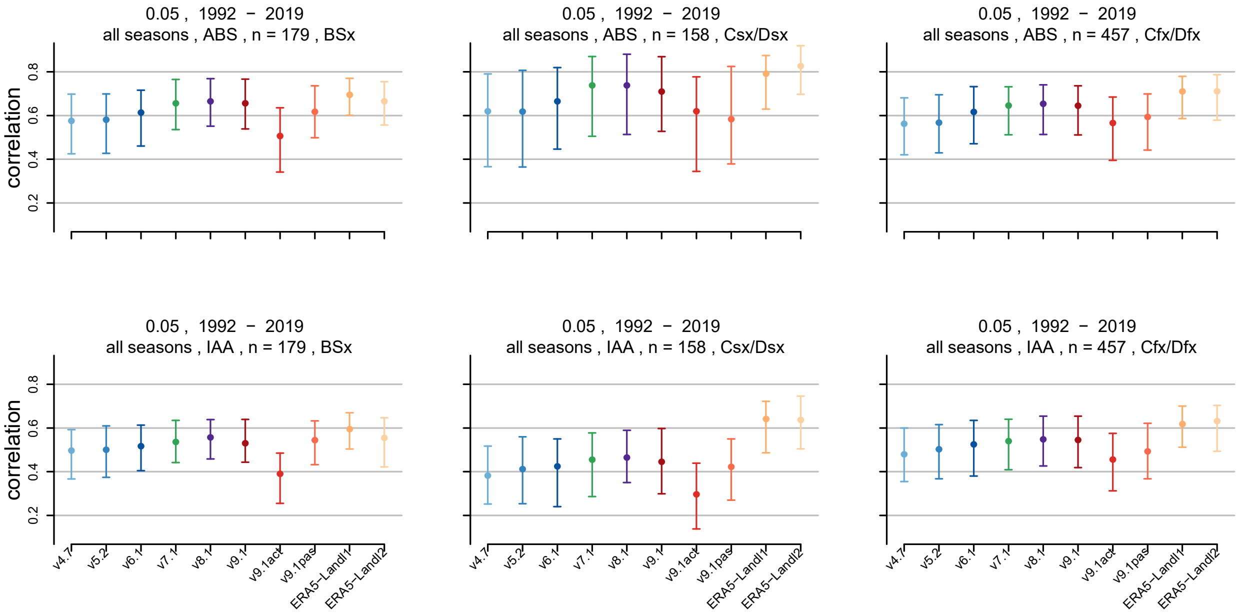

Figure 18: Correlation of the gridded soil moisture products (ESA CCI SM v04.7, v05.2, v06.1, v07.1, v08.1 and v09.1 COMBINED, ACTIVE (9.1act) and PASSIVE (v9.1pas) for v09.1, as well as ERA5-Land (layers 1 and 2)) as compared to in-situ station observations (5 cm depth) for three combinations of Köppen-Geiger classes (BSx - arid, Csx/Dsx - temperate/continental summer dry, Cfx/Dfx - temperate/continental without dry season). (Top row) Absolute values of soil moisture (ABS); (bottom row) inter-annual anomalies (IAA). Shown is the median and IQR of the correlations, n denotes the number of stations underlying the distributions.

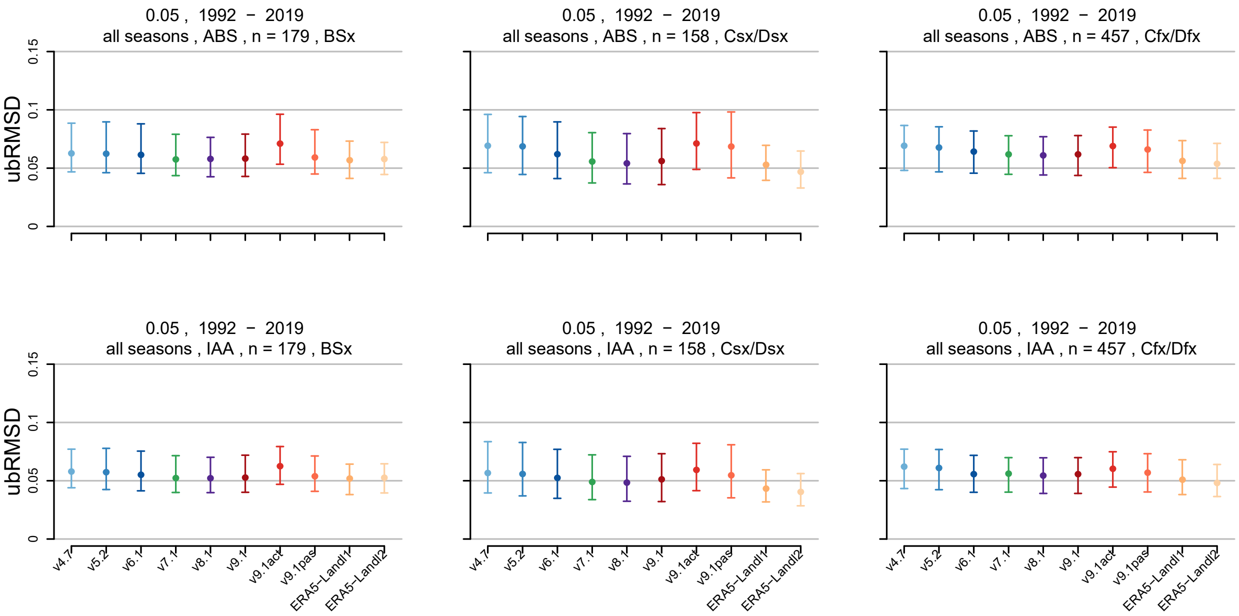

Figure 19: As Figure 18, but showing ubRMSD.

Focusing on the US only where spatial coverage with in-situ stations is most dense (Figure 20), correlation is highest for the absolute values and drops considerably for the anomalies. We find that the spatial pattern of the ESA CCI SM COMBINED correlations is rather scattered for the absolute values, and there are no clear areas in which the product agrees either very well or very poorly with in-situ soil moisture. For the anomalies, the ESA CCI SM correlations appear lower in the north-eastern of the region, which is likely related to complex topography. This is not the case for ERA5-Land layer 1.

There is a slight increase in correlation for each subsequent ESA CCI SM release, most notable when comparing v4.7 to v09.1. ERA5-Land layer 1 shows better agreement with in-situ soil moisture than ESA CCI SM, for both absolute values and anomalies.

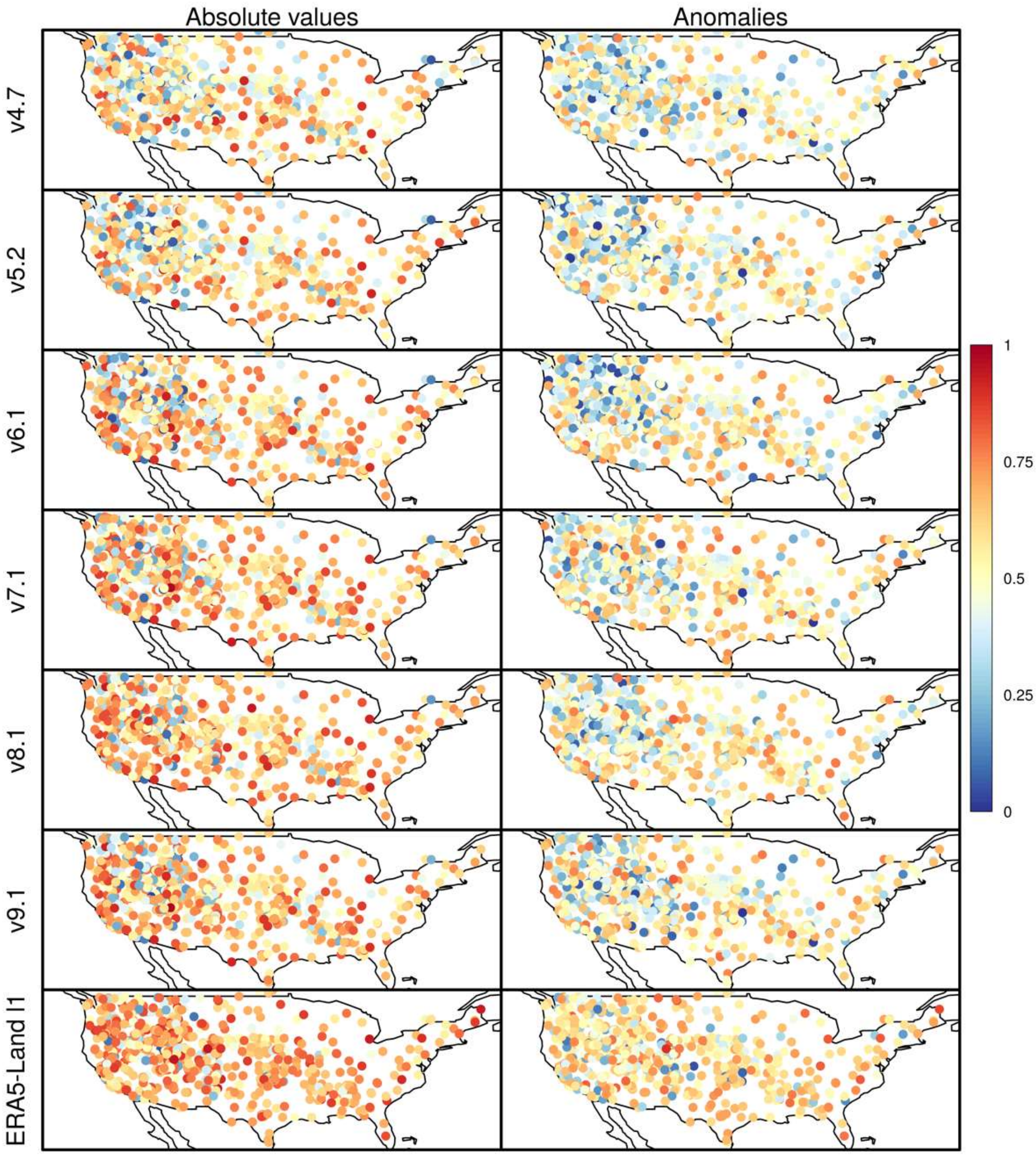

Figure 20: Correlation between in-situ soil moisture and ESA CCI SM for versions v04.7, v05.2, v06.1, v07.1, v08.1 and v09.1 COMBINED, as well as ERA5-Land soil moisture layer 1 (ERA5-Land l1, 0-7 cm), for absolute soil moisture (left) and the anomalies (right) and the period 1992-2019.

5.2.3 Temporal subsets and product evolution

Figure 21 shows the (significantly positive, $p < 0.05$) correlations of the different ESA CCI SM releases, as well as ERA5-Land layer 1 compared to in-situ stations (extended set of stations, see Section 5.2.1) in the US for different temporal subsets (i.e., 1999-2002, 2003-2006, 2007-2010, 2011-2014, 2015-2018 and 2019-2022, as well as 1999 up to the end of the individual time series).

The overall correlations for ESA CCI SM appear higher in the earliest period, with a drop during 2003-2006 and subsequent increase towards later periods. This behaviour is in particular visible for autumn (not shown). The correlations of ERA5-Land are more stable over time. The ESA CCI SM releases show a general increase in performance with data releases, pointing to the increasing maturity of the product. This is in particular the case for later periods and when considering earlier versions, while the improvements from v08.1 to v09.1 are comparably small. As for the global validation with ISMN, the PASSIVE and ACTIVE products of v09.1 often show lower skill compared to the COMBINED product. An exception is the first time slice, where the ACTIVE product of v09.1 shows better agreement with in-situ observations than the COMBINED and PASSIVE products (though based on a reduced set of in-situ stations).

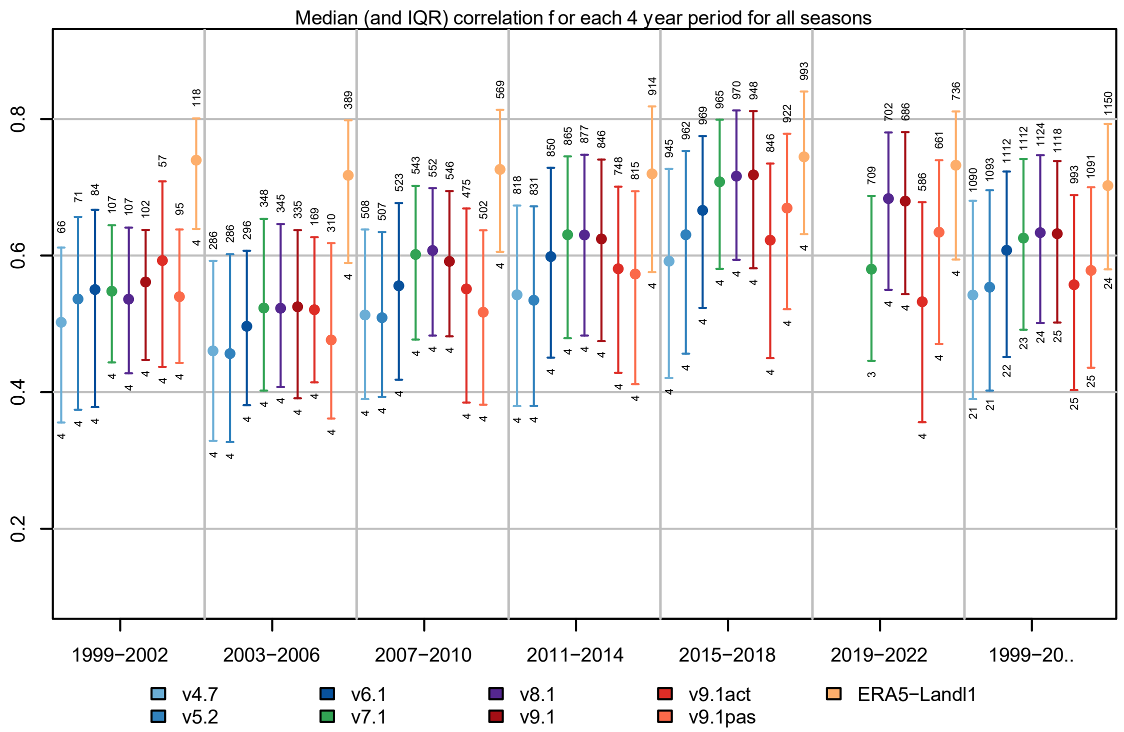

Figure 21: Correlation of the gridded soil moisture products as compared to in-situ station observations in 5 and 10 cm depth for the full year for the US. Subdivided in consecutive 4-year periods (1999-2002, 2003-2006, 2007-2010, 2011-2014, 2015-2018 and 2019-2022) as well as for the longest period data is available (1999-20..). Note that in this case, data is not masked for common data availability. Whiskers show the median and the IQR. Above indicated the number of stations correlations were calculated for that comply to the following criteria: at least 10% of the time-series is not NA, p-value < 0.05, and the calculated correlation is positive. And below indicated the number of years considered. In addition to the major post-v3 releases of ESA CCI SM COMBINED, ACTIVE and PASSIVE products are shown in case of v09.1 (denoted v9.1act and v9.1pas).

5.2.4 The influence of measuring depth

ESA CCI SM represents soil moisture in only the top few millimeters to centimeters of the soil [*Dorigo et al.*, 2012; *Dorigo et al.*, 2017]. To determine the influence of measuring depth on the correlation we differentiate between in-situ measurements at 5 and 10 cm depth, see Figure 22. As noted above, the near-surface measurements may be more prone to errors due to their vicinity to air [*Mittelbach et al.*, 2012]. Considering also the 10 cm measurements increases the robustness of the comparisons and may help to detect systematic degradations of the 5 cm sensors. For each major post-v3 release of ESA CCI SM COMBINED as well as for ERA5-Land (layers 1 and 2), we distinguish between three different regions (US, EU, and AUS) and show the results for the absolute values (top panel) as well as the anomalies (bottom panel). Circles denote correlations with in-situ measurements taken at 5 cm depth, and triangles at 10 cm depth.

ESA CCI SM: For the US and Europe, there is a large spread in the derived correlations, likely due to the large spread in climate conditions that the stations are located in. For Australia, the spread is much smaller, there are far fewer stations here and they are all located in the south-eastern part of the continent. For the US, the absolute values show correlations for the ESA CCI SM releases ranging between 0.1 to over 0.9 for the comparison with the 5 cm in-situ measurements, and between 0.1 to 0.8 (for later versions) for the 10 cm measurements, with the median correlation for the shallower 5 cm in-situ measurements being consistently higher. For Europe, the 5-cm correlations are similar as for the US with median values of around 0.6, but slightly less spread. The 10-cm median correlations for Europe tend to be higher than in the US, resulting in a less clear distinction between the 10 cm and 5 cm correlations in this region (though the median correlations for the shallower in-situ measurements still tend to be higher). The overall highest correlations are found in Australia, with over 0.7 for the median. Again, the correlations are lower for 10 cm depth.

For the anomalies, the distinction between the 5 cm and the 10 cm correlations follows similar patterns as for the absolute values, but with overall lower correlations.

ERA5-Land: Consistent with ESA CCI SM, absolute values of ERA5-Land layer 1 (l1) and layer 2 (l2) show higher correlations with in-situ measurements at 5 cm depth than at 10 cm depth for the US and Europe. For Australia, the pattern is reversed, both for absolute values and the anomalies and correlation with measurements taken at 10 cm are higher in this region. The median correlation for 10 cm is also slightly higher over Europe for the anomalies of ERA5-Land l2. The range of the correlations of ERA5-Land is similar to ESA CCI SM v09.1 (i.e., also going up to over 0.9 for the absolute values), and with overall mostly higher median correlations.

Overall, these results are according to expectations and do not indicate widespread or systematic degradations of the 5 cm compared to the 10 cm in-situ measurement.

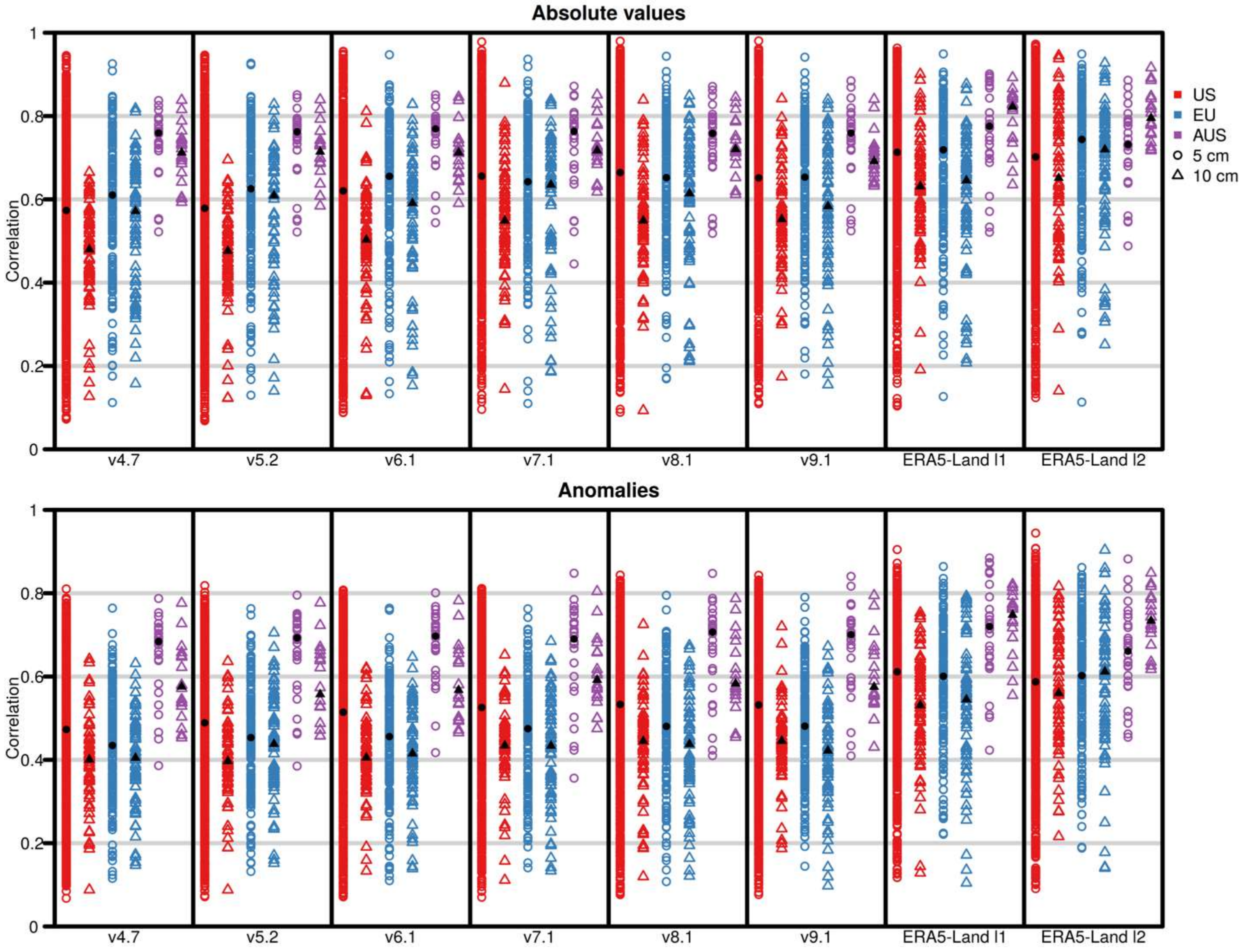

Figure 22: Correlation between in-situ measurements and ESA CCI SM v04.7, v05.2, v06.1, v07.1, v08.1 and v09.1, as well as ERA5-Land soil moisture layer 1 and 2 for the absolute soil moisture values (top) and the anomalies (bottom). For each product, we distinguish between 3 regions US, EU, and AUS (red, blue and purple, AF has insufficient data coverage), and the correlation at 5 cm depth (circles) and 10 cm depth (triangles) over the 1992-2019 time period. The same number of stations is taken into account for the individual distributions of the top and bottom panels. The black circles/triangles represent the respective median values.

5.2.5 The influence of land cover

Figure 23 shows the correlations of ESA CCI SM v04.7, v05.2, v06.1, v07.1, v08.1 and v09.1 (COMBINED products), as well as ERA5-Land layer 1 with the in-situ measurements over the US for absolute values and their inter-annual anomalies, differentiating between grassland (orange) and forest (green) sites (based on the land-cover information of the ISMN stations). As above, correlations for the anomalies are lower compared to the absolute values for all products. For ESA CCI SM, there is mostly a notably higher correlation for grassland sites than for forest sites, both for the absolute values as well as the anomalies. This is related to the reduced retrieval quality over more densely vegetated areas. For ERA5-Land, such a distinction in the skill between the two land cover types is also visible, but to a lesser degree.

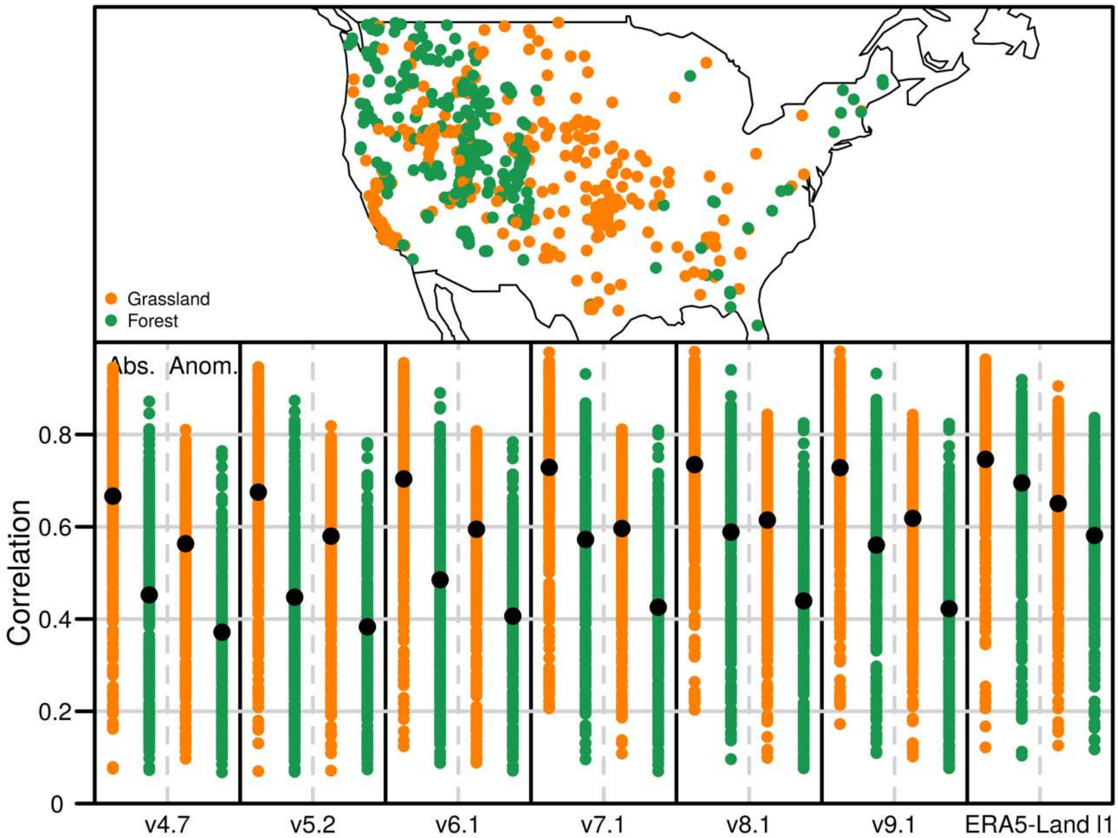

Figure 23: Correlation between in-situ measurements at 5 cm depth and ESA CCI SM v04.7, v05.2, v06.1, v07.1, v08.1 and v09.1, as well as ERA5-Land soil moisture layer 1 over the 1992-2019 time period, differentiating between grassland (orange) and forest (green) sites for absolute soil moisture values and anomalies. Black dot denotes the median value.

5.2.6 Summary

- Spatially scattered pattern in correlations, no clear areas in which the ESA CCI SM products agree either very well or very poorly with in-situ soil moisture. Though, highest correlations are found in Australia.
- ESA CCI SM shows mostly higher correlations with in-situ measurements at 5 cm depth than at 10 cm depth. For ERA5-Land this distinction is reversed in Australia.
- Also, ESA CCI SM shows higher correlations with in-situ measurements over grassland sites than over forest sites. For ERA5-Land this difference is less pronounced.
- ERA5-Land reanalysis soil moisture on the average shows better agreement with the in-situ data compared to ESA CCI SM. However, ESA CCI SM shows a general increase in skill with subsequent major releases particularly when considering earlier versions, pointing to the increasing maturity of the remote sensing product. The latest ESA CCI SM v08.1 and v09.1 show similar agreement with in-situ data.

5.3 Long-term trends

5.3.1 Datasets and trend calculation

In this section, temporal trends of aggregated yearly mean soil moisture are analysed for different time periods. As in previous sections, major product releases of ESA CCI SM are considered and compared to the ERA5-Land and the MERRA-2 reanalysis soil moisture (surface layer). In addition, also GLDAS-Noah (for trends from 2000 onwards) as well as an gap-filled version of the v09.1 COMBINED product [available from 1991 onwards; *Preimesberger et al.*, 2024] is included in the analysis. Theil-Sen trend estimates for the 1988-2010, 1992-2022, and 2000-2022 time periods are presented (Figure 24 - Figure 26), and significance is determined using Mann-Kendall trend tests (p-value < 0.05 for significant trends).

5.3.2 Results

Significant trends in all major product versions (i.e., COMBINED products of ESA CCI SM v0.1, v02.2, v03.3, v04.7, v05.2, v06.1, v07.1, v08.1 and v09.1) are only partly consistent for the common 1988-2010 time period (Figure 24). In particular, a large-scale tendency for more widespread wetting trends in the northern mid-latitudes is visible with later product versions. The drying trends in Siberia (most pronounced in v04.7 and v05.2) partly turn into wetting trends. Also, the original significant wetting trend in southern Africa disappears with the later product releases, while Patagonia starts to experience wetting trends. Over Australia, the widespread drying trend present in v0.1 also mostly disappears and partly turns into a wetting trend in v07.1 to v09.1.

Comparing the last three product releases of ESA CCI SM (v07.1 to v09.1, COMBINED products), significant trend patterns appear mostly similar. ESA CCI SM v09.1 shows slightly more pronounced drying trends in parts of East Asia.

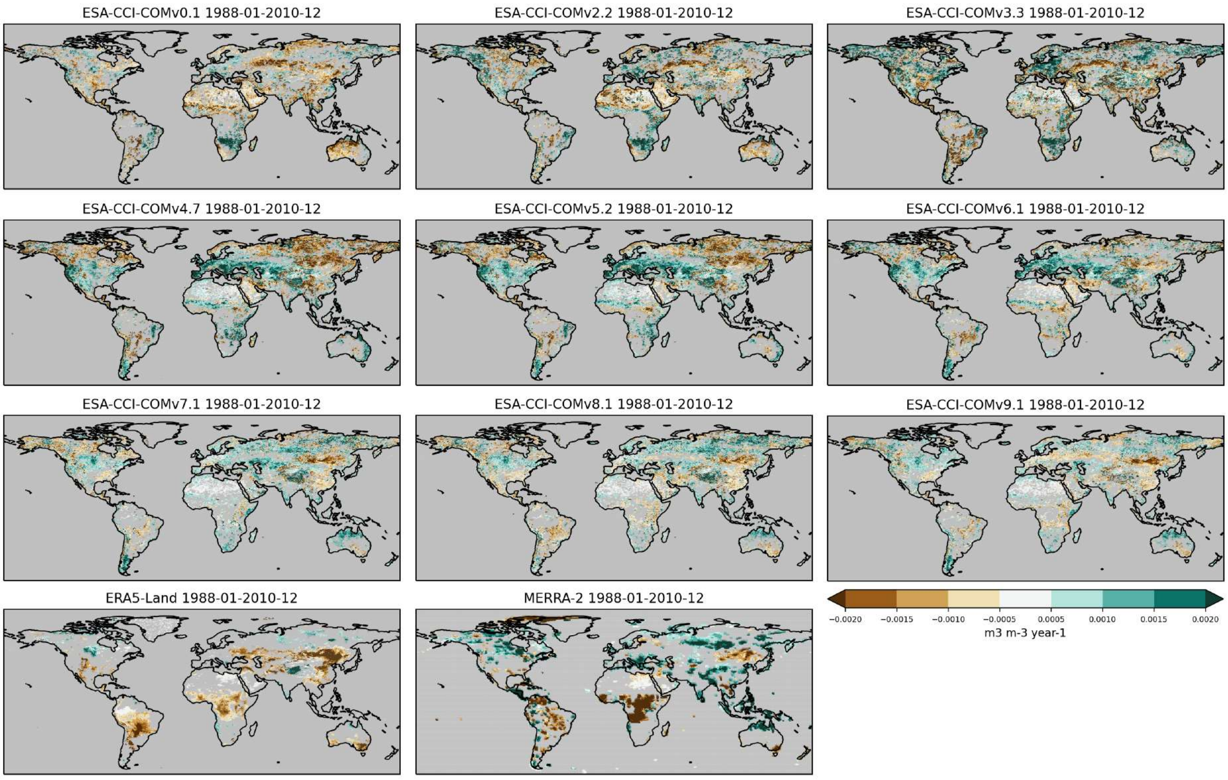

Figure 24: Evolution of 1988-2010 trends with the major product releases ESA CCI SM (v0.1, v02.2, v03.3, v04.7, v05.2, v06.1, v07.1, v08.1 and v09.1 COMBINED products), and in comparison to ERA5-Land and MERRA-2. Theil-sen trend estimate based on yearly mean surface soil moisture (m^3 m^{-3} per year). A Mann-Kendall test with a false rejection rate (or alpha value) of 0.05 was performed to mask out regions where no significant trend is present.

The significant trends of ESA CCI SM v09.1 COMBINED, and of the ERA5-Land and MERRA-2 reanalysis products are also diverse and only partly consistent. In particular, ERA5-Land shows a predominance of significant drying trends for the 1988-2010 and 1992-2022 time periods, while ESA CCI SM v09.1 COMBINED and MERRA-2 show more mixed significant drying and wetting trends for these periods (Figure 24 and Figure 25). Differences in the distribution of significant trends over the 1992-2022 period are also visible between the COMBINED, ACTIVE and PASSIVE products of both ESA CCI SM v09.1 and v08.1. In particular, the PASSIVE products display drying trends in Europe, southern USA and parts of Asia and South America, while the COMBINED products display non-significant or weaker drying trends in these regions, and the ACTIVE products mostly and strong wetting trends (Figure 25). On the other hand, the widespread significant wetting trends of the PASSVE products present in southern Africa and northeast Brazil during 1992-2022 are mostly absent in the ACTIVE or slightly negative in the COMBINED products of v8.1 and v9.1.

For the 2000-2022 period, trend magnitudes become intensified in the COMBINED products compared to 1992-2022. The PASSIVE products display less widespread significant drying trends for this recent period (and corresponding larger fractions of positive trends), while the

COMBINED products show more widespread drying trends, and the ACTIVE products mostly strong wetting trends. Similar as for the other periods, ERA5-Land displays more significant drying trends for 2000-2022, while MERRA-2 (except for larger parts of the Southern Hemisphere) shows widespread and strong wetting trends. In case of GLDAS-Noah, widespread and strong negative trends are present for this period, except for parts of Asia. These are exceeding the negative trends seen in ERA5-Land.

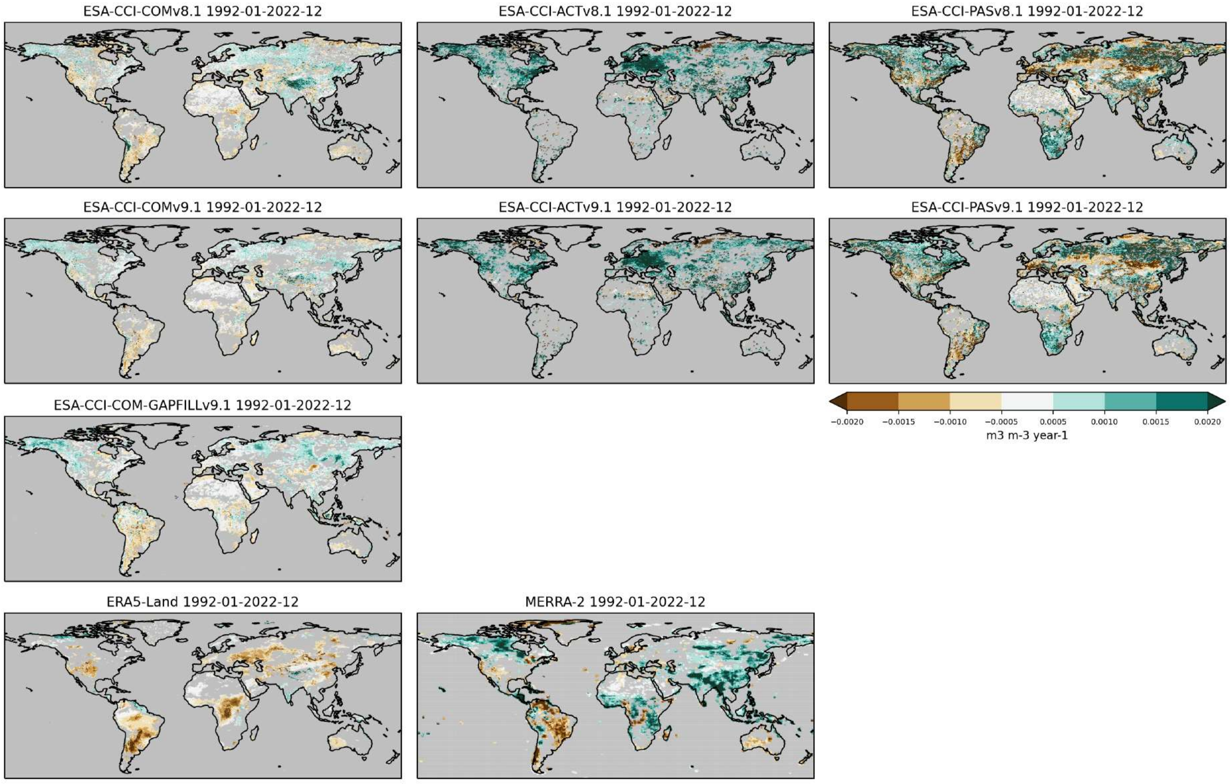

Figure 25: As Figure 24, but for the long-term 1992-2022 trends of v09.1 and v08.1 COMBINED, ACTIVE and PASSIVE, and in comparison to ERA5-Land and MERRA-2. For v09.1, also the gap-filled research product based on COMBINED is displayed.

Comparing the v09.1 COMBINED product with its gap-filled version, trend patterns appear mostly similar. For the latter, a tendency for partly stronger wetting trends in some areas of the northern mid to high latitudes can be observed for both the 1992-2022 and 2000-2022 periods as a result of the increased data coverage (Figure 25 and Figure 26). Similar effects of the gap-filling have also been observed by e.g., *Bessenbacher et al.* [2023; using a different approach for gap-filling], but acting in the opposite direction (i.e., reduction of wetting trends in this region in the gap-filled data; cf. Figure 8 therein). It should be noted, however, that apart from the gap-filling approach applied, differences in these effects may also arise from differences in the product version used (i.e., v07.1 in the aforementioned study vs. v09.1 here), the application of linear trends vs. Theil-sen trends respectively, and slightly different time periods considered. Overall, the artefacts of incomplete data coverage tend to be most pronounced when looking at regional averages [*Bessenbacher et al.*, 2023].

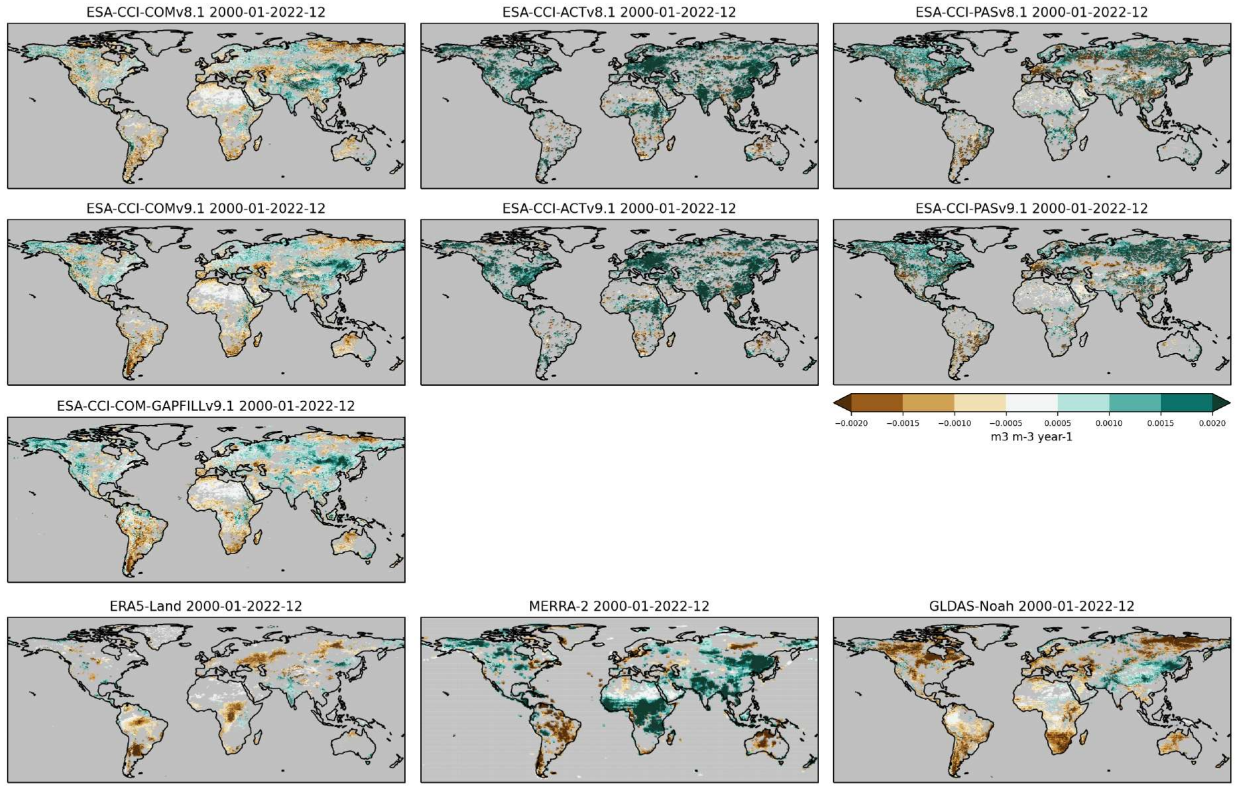

Figure 26: As Figure 25, but for the recent 2000-2022 trends and including GLDAS-Noah.

5.3.3 Summary

- The representation of long-term significant trends over the common 1988-2010 period shows changes in magnitude and sign with the evolution of ESA CCI SM (COMBINED product) in several large-scale regions.
- Trends in the last three product releases of ESA CCI SM COMBINED (v07.1 to v09.1) appear mostly similar.
- Significant trend patterns partly diverge between the ESA CCI SM COMBINED, and the underlying ACTIVE and PASSIVE products, as well as compared to reanalysis and land-surface model products. ERA5-Land and particularly GLDAS-Noah show widespread negative trends, while MERRA-2 and the ACTIVE products show more widespread positive trends. Trends in the COMBINED and PASSIVE products appear more mixed.

6 Conclusions

Based on the various verification and validation activities described in this PVIR, the current ESA CCI SM v09.1 product is generally suitable for representing the spatio-temporal evolution of surface soil moisture (in particular, its temporal dynamics). When compared to in-situ measurements, the ESA CCI SM shows a general increase in skill with subsequent major data releases, which points to the increasing maturity of the product. The latest v08.1 and v09.1 show stable agreement compared to the in-situ data, this is the case for the COMBINED as well as the ACTIVE and PASSIVE products.

Within the ESA CCI SM v08.1, the COMBINED product performs best in terms of all considered metrics, which clearly shows the benefit of merging active and passive remote sensing for global surface soil moisture.

Large uncertainties remain in the representation of long-term temporal trends, which display distinct and partly diverging patterns among the major product releases of ESA CCI SM COMBINED and the underlying ACTIVE and PASSIVE products, as well as when compared to reanalysis and land-surface model products.

Finally, the potential of data assimilation for adding value to the ESA CCI SM product has been noted in previous PVIRs, e.g., by providing soil moisture information at higher spatial resolution in the horizontal, and in the vertical (e.g., providing information on root zone soil moisture). This is especially relevant for regions where high-quality precipitation data sets are lacking, here the ESA CCI SM product can provide valuable additional information of the state of the land surface. Various workshops and meetings within the ESA CCI for soil moisture have identified the importance of root zone soil moisture information for studies of the climate system, including the hydrological and carbon cycles.

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