ESA Climate Change Initiative Plus - Soil Moisture

Product Validation and Intercomparison Report (PVIR)

Supporting Product version v06.1

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Submitted by

EODC Earth Observation Data Centre for Water Resources Monitoring GmbH

in cooperation with

TU Wien, VanderSat, ETH Zürich, and CESBIO

This document forms the deliverable D4.1 Version 2, Product Validation and Intercomparison Report (PVIR) and was compiled for the European Space Agency (ESA) Climate Change Initiative Plus Soil Moisture Project (ESRIN Contract No: 4000126684/19/I-NB: "ESA CCI+ Phase 1 New R&D on CCI ECVS Soil Moisture").

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

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Acronyms

ABS	Absolute soil moisture
AMSR-E	Advanced Microwave Scanning Radiometer - Earth Observing System
ASAR	Advanced Synthetic Aperture Radar
ASCAT	Advanced SCATterometer
ATBD	Algorithm Development Document
CAL-VAL	Calibration and validation
CDF	Cumulative Distribution Function
CCI	Climate Change Initiative
DA	Data Assimilation
ECMWF	European Centre for Medium Range Weather Forecasts
ENVISAT	Environmental Satellite
ECV	Essential Climate Variable
CCI SM	Soil moisture time series developed in framework of ESA CCI
EO	Earth Observation
ERA	ECMWF Re-Analysis
ESA	European Space Agency
ISMN	International soil moisture network
LSM	Land surface model
LTA	Long-term anomaly of soil moisture
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
PSD	Product Specification Document
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
STA	Short-term anomaly of 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 (1978-2020) soil moisture time series (ESA CCI SM v06.1) 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 v06.1 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); R (Pearson's correlation coefficient) and ubRMSD (unbiased root-mean-square-difference) are calculated and analysed. Validations are performed globally and after bias correction by matching the mean and standard deviation of each ESA CCI SM time series to that of the reference series. For inter-comparison between versions, only the common observations are used.

The evaluation of ESA CCI SM v06.1shows differences compared to the last public version. Differences are found in terms of temporal coverage (due to the dataset extension) but also in terms of flagging of input datasets. The comparison against ERA5 has also shown some improvements in correlation in the same areas.

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 and ERA-Interim/Land soil moisture reanalyses at 0.25° resolution (Section 5.2). In this validation process, the current release v06.1 is also set into perspective to previous major releases of ESA CCI SM from v0.1 up to v05.2. The evaluation uses the two top layers of the ERA 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.MERRA-2 is also 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 consistently 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 clear for the comparison with the ERA5-Land reanalysis.

Overall, the ESA CCI SM v06.1 product releases show increasing correlations with in-situ data with the evolution of the product pointing to the mature state of the product, and clear improvements between v06.1 and v05.2 are in particular visible for the more recent period. However, remaining uncertainties exist 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 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 1 - NEW R&D ON CCI ECVS Soil Moisture Project Contract No: 4000126684/19/I-NB.

[AD-2] Climate Change Initiative Extension (CCI+) Phase 1 New R&D on CCI ECVs, Statement of Work, ESA Earth Observation Directorate, ESA-CCI-EOPS-PRGM-SOW-18-0118.

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), revision 3, version 2.6, 29 Nov. 2018

[RD-02] Algorithm Theoretical Basis Document (ATBD), v6.1, Mar. 2021

[RD-03] Soil Moisture CCI Product User Guide (PUG), v6.1, Mar. 2021

[RD-04] Climate Research Data Package (CRDP), v6.1, Mar. 2021

[RD-05] Product Validation Plan (PVP), version 2, Nov. 2020

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 v06.1 time series is provided in the Algorithm Development Document (ATBDv6.1), as well as the Product User Guide (PUGv6.1), 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

The following table shows an overview of the datasets used for the validation of the ESA CCI SM product. For details on the single ESA CCI SM product versions, please refer to the CDRP [RD-04].

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	1991-2020	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	1988-2019	Global
ERA-Interim/Land	ECMWF	Land surface model reanalysis	Reanalysis data for volumetric soil water at different levels of the soil profile	1991-2010	Global
ERA5	ECMWF	Atmospheric reanalysis	Reanalysis data for volumetric soil water at different levels of the soil profile	2007-2019	Global
MERRA-2	NASA	Atmospheric reanalysis	Reanalysis data for volumetric soil water at different levels of the soil profile	1988-2019	Global

5 Verification and validation results

The following sections present the verification and validation results of the ESA CCI SM v06.1 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 ensure the physical plausibility of the ESA CCI SM products generated and to ensure that the scientific developments have positively contributed to the product. The new break-adjusted product of ESA CCI SM v06.1 COMBINED [based on *Preimesberger et al.*, 2021] is also assessed for completeness and differences to the non-break-adjusted product.

5.1.1 Datasets

ESA CCI SM

In addition to the newly generated datasets of ESA CCI SM v06.1, the previous public release (v05.2) has been used[1]. All three respective products of ESA CCI SM (ACTIVE, PASSIVE, COMBINED) have been analysed, however, only a subset of these results are 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 2019-12-31 is used.

5.1.2 Dataset Completeness

Figure 1 shows the fractional coverage of ESA CCI SM COMBINED observations over time and latitude and Figure 2 shows the difference between the fractional coverage of v06.1 and v05.2. Note: the same plot is shown for the ACTIVE and PASSIVE products in Figure 5 and Figure 6 respectively at the end of this section for the benefit of data users along with the associated maps.

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. In addition, around the equator, coverage is reduced due to high vegetation cover in many areas where soil moisture cannot be reliably retrieved. These comments are applicable to all data products (COMBINED, PASSIVE and ACTIVE; Figure 1, Figure 5 and Figure 6 respectively).

In terms of the difference to the previous product (shown in Figure 2), it can be seen that there is an increase in the fraction of valid observations where new datasets have been utilised, for example where the TMI dataset has been extended. However, there is a reduction where the improved snow flagging has been implemented.

[1] Note that the v05.2 dataset runs to 2019-12-31 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.

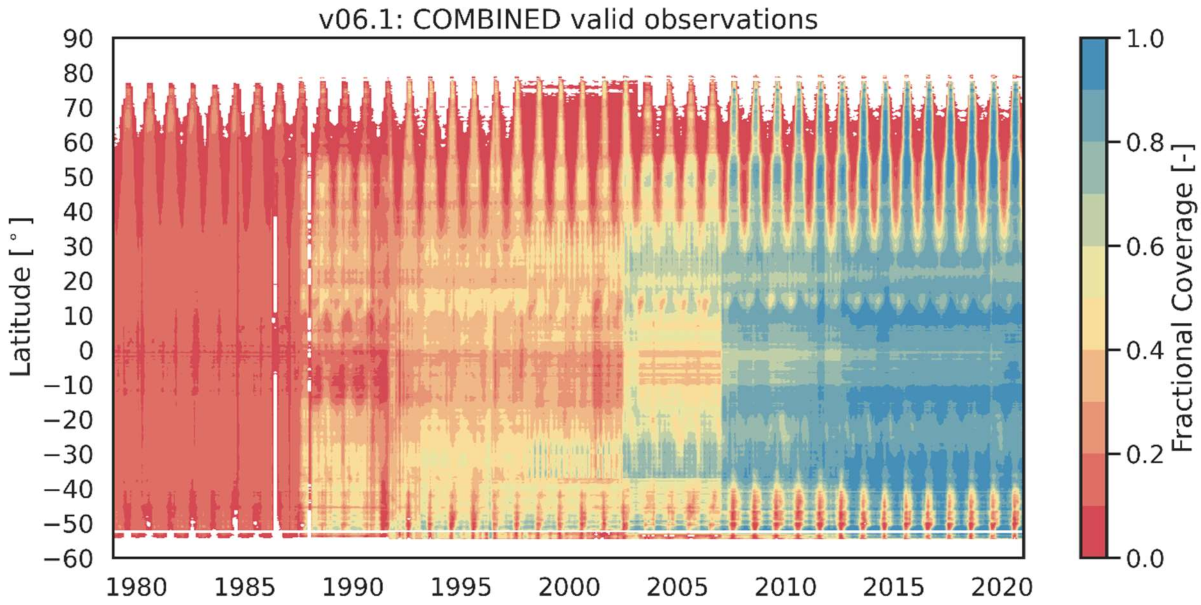

Figure 1 : Hovmöeller diagram of the fractional number of valid observations per month in the Soil Moisture variable of ESA CCI SM v06.1 COMBINED product. Note: areas of high vegetation are masked out from the monthly / latitude aggregation.

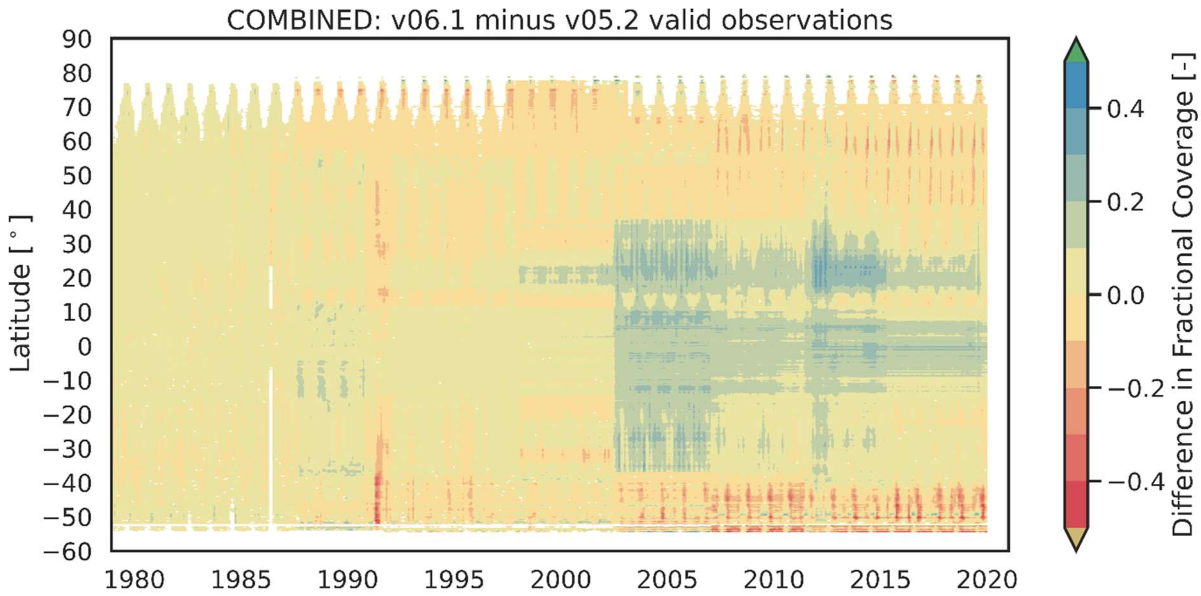

Figure 2 : Hovmöeller diagram of the difference in the fractional number of valid observations per month in the Soil Moisture variable of ESA CCI SM v06.1 COMBINED product compared to the ESA CCI SM v05.2 COMBINED product.

The spatial distribution of the coverage is provided in Figure 3 for the period 2007-01-01 to 2020-12-31 (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 as well as bare soils.

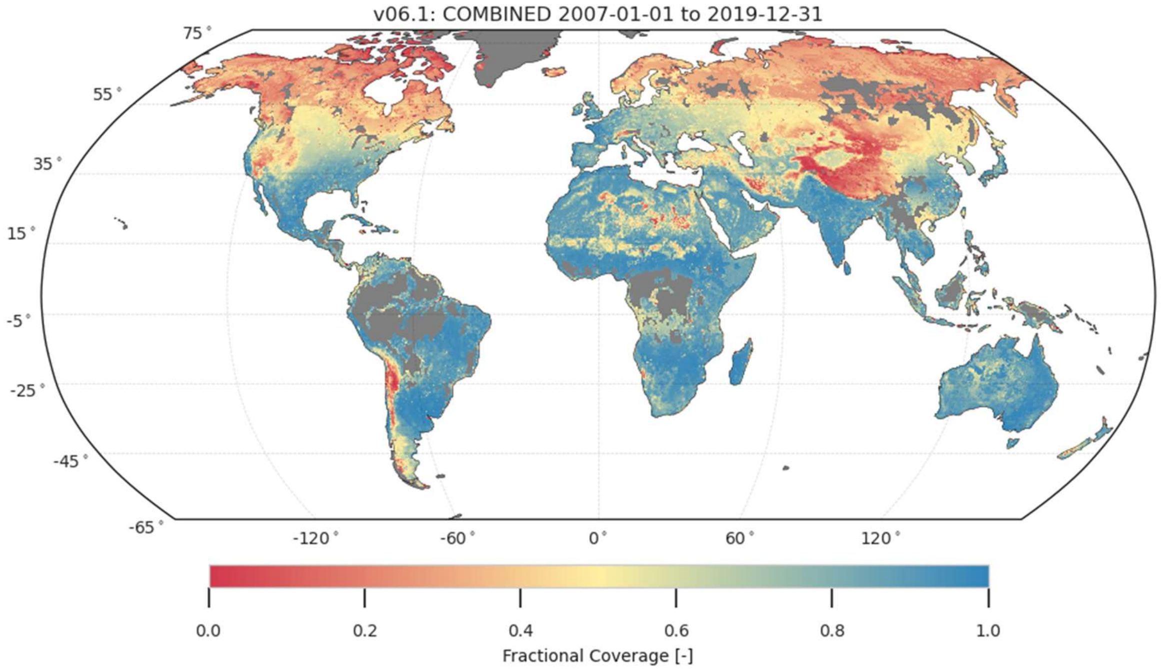

Figure 3 : Spatial fraction of valid observations in the Soil Moisture variable of ESA CCI SM v06.1 COMBINED product for the period 2007-01-01 to 2019-12-31. Note: areas of high vegetation are masked out and appear as grey.

The improvements in snow flagging both for ASCAT and LPRM (passive) [*van der Vliet et al.*, 2020] are a key feature of the new ESA CCI SM v06.1 product and are reflected in the comparison of the coverage map to the results from v05.2 (Figure 4). In addition, it can be seen that v06.1 provides more valid observations than v05.2 in some areas, particularly deserts. This is due to the increased number of sensors used in the period considered, i.e., GPM, FY-3B and the extension of TMI up to 2015.

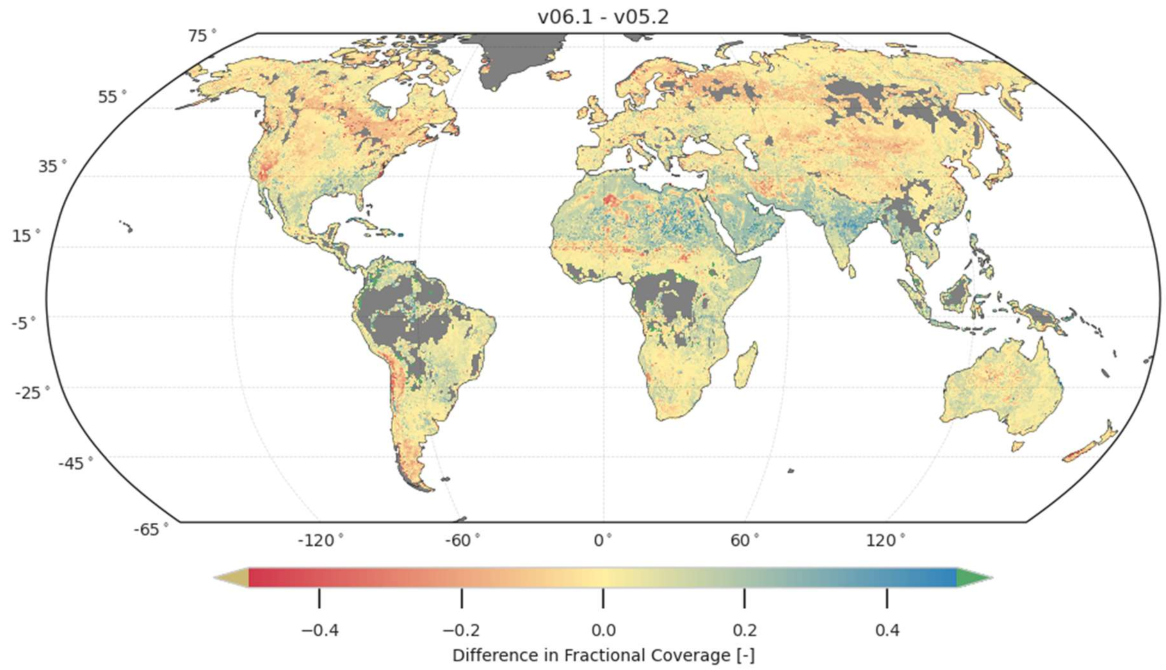

Figure 4 : Difference in the spatial fraction of valid observations in the Soil Moisture variable of ESA CCI SM v06.1 COMBINED and v05.2 for the period 2007-01-01 to 2019-12-31. Blue represents an increase in valid observations in the new (v06.1) product.

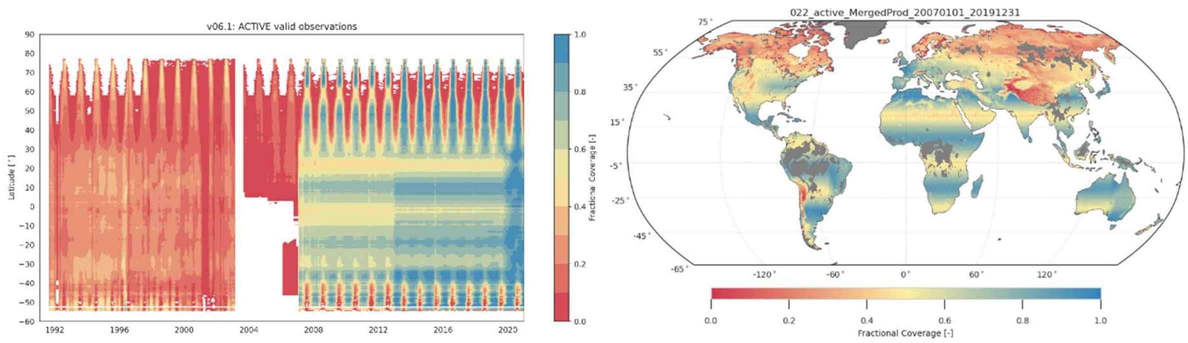

Figure 5 : Hovmöeller diagram of the fractional number of valid observations per month in the Soil Moisture variable of ESA CCI SM v06.1 ACTIVE product (left) with the spatial distribution of valid observations for the period 2007-01-01 to 2019-12-31 (right). Note: areas of high vegetation are masked out from the monthly / latitude aggregation.

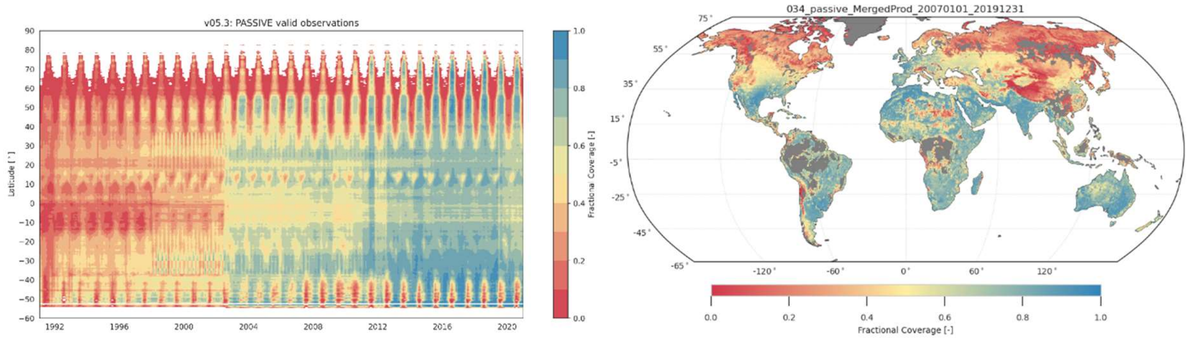

Figure 6 : Hovmöeller diagram of the fractional number of valid observations per month in the Soil Moisture variable of ESA CCI SM v06.1 PASSIVE product (left) with the spatial distribution of valid observations for the period 2007-01-01 to 2019-12-31 (right). Note: areas of high vegetation are masked out from the monthly / latitude aggregation.

5.1.3 Dataset Uncertainty

Figure 7 shows changes in the uncertainty variable in ESA CCI SM v06.1 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 **Error! Reference source not found.** that the uncertainty (which is calculated per sensor period) reduces over time with the most recent periods showing uncertainty of below 0.01.

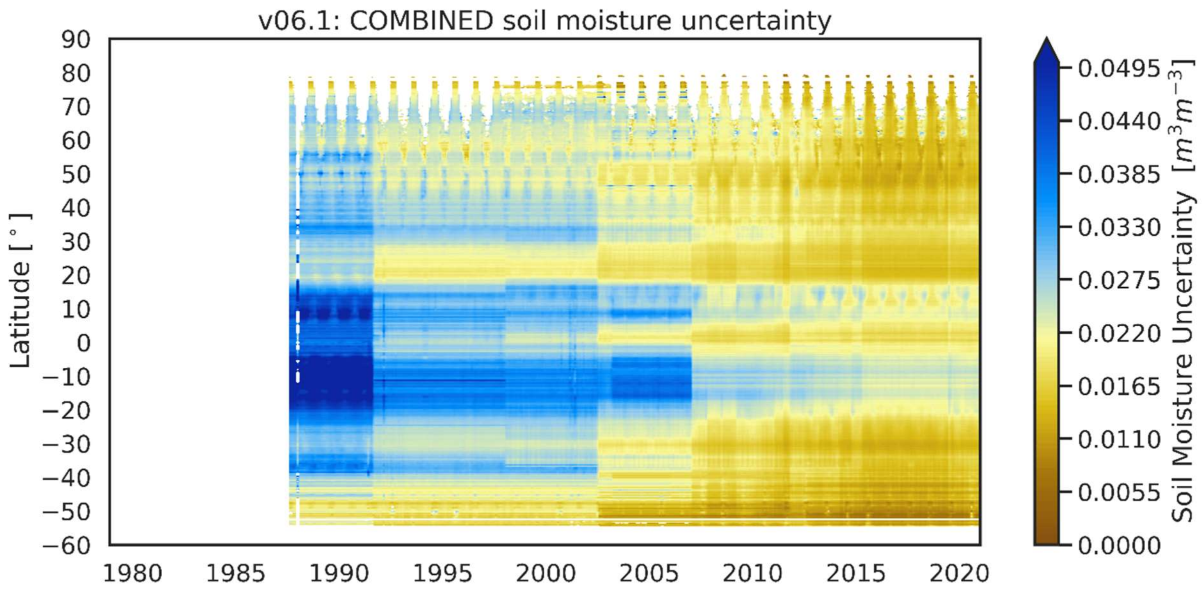

Figure 7: Monthly soil moisture uncertainty in ESA CCI SM v06.1 COMBINED. Note: areas of high vegetation are masked out from the monthly / latitude aggregation.

5.1.4 Soil Moisture Statistics

The mean and standard deviation of the ESA CCI SM v06.1 COMBINED product (Figure 8 and Figure 9) have been calculated for the period 2007-01-01 to 2019-12-31 and compared to the same results from the v05.2 COMBINED product (Figure 10).

The spatial patterns shown for both the mean and standard deviation are as expected and we see from the comparison that the statistics have not significantly changed between v06.1 and v05.2.

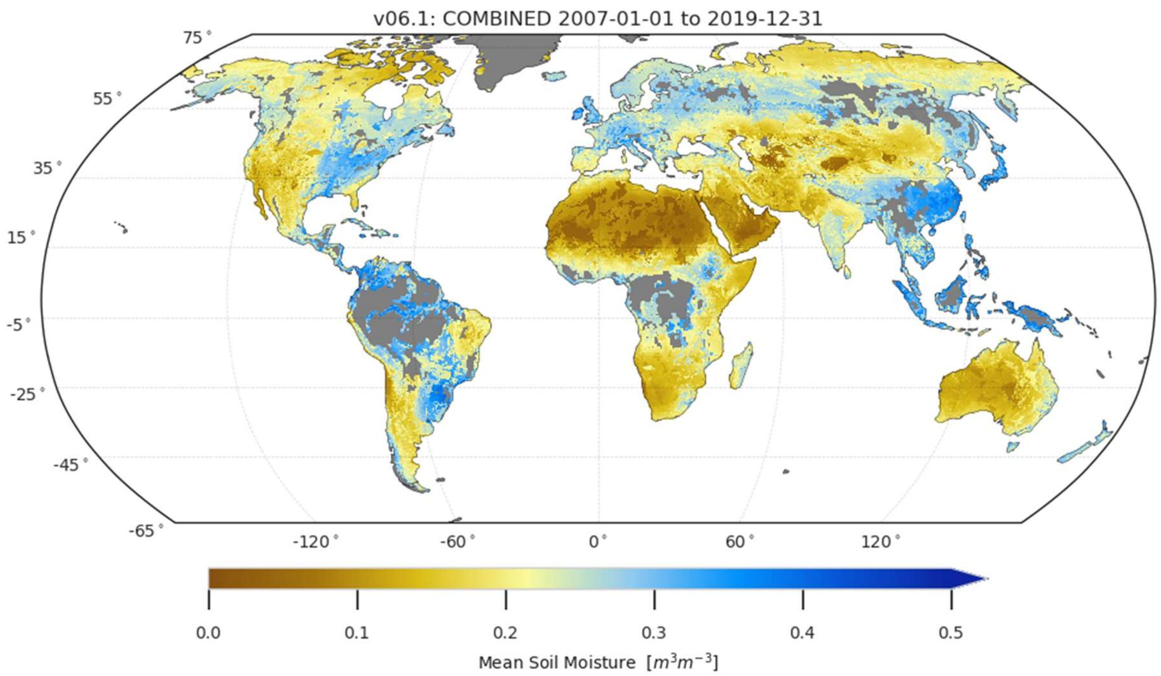

Figure 8: Mean soil moisture for the ESA CCI SM v06.1 COMBINED product for the period 2007-01-01 to 2019-12-31.

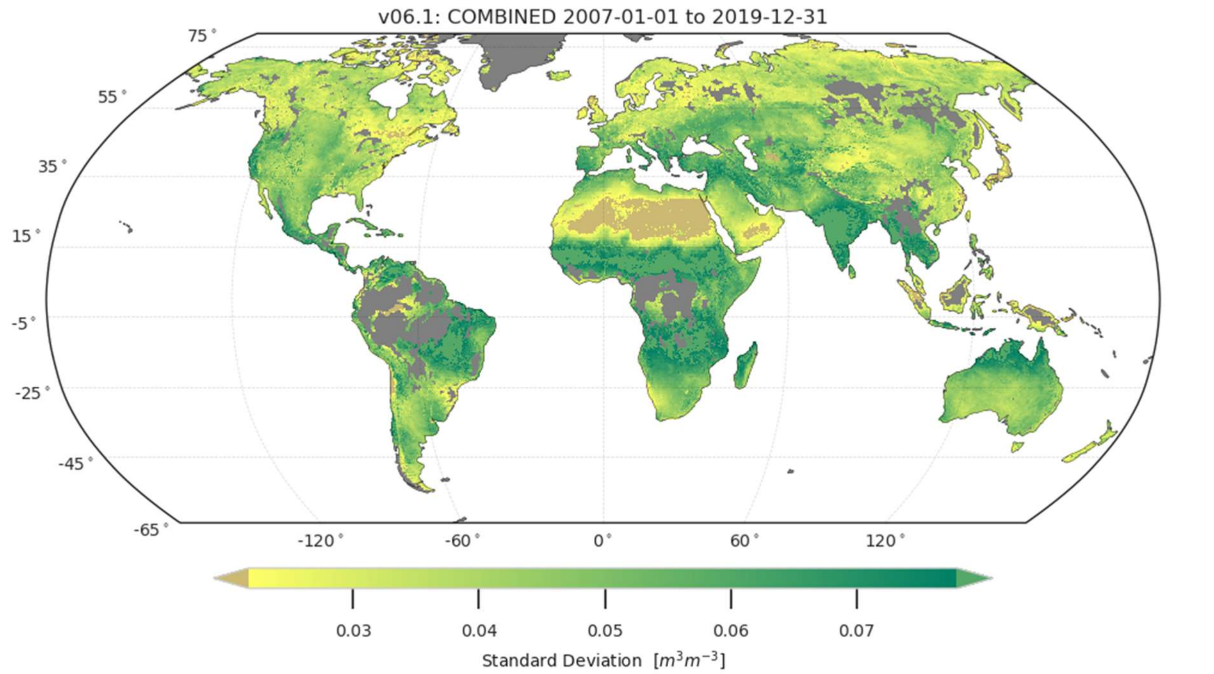

Figure 9: Standard deviation of soil moisture for the ESA CCI SM v06.1 COMBINED product for the period 2007-01-01 to 2019-12-31.

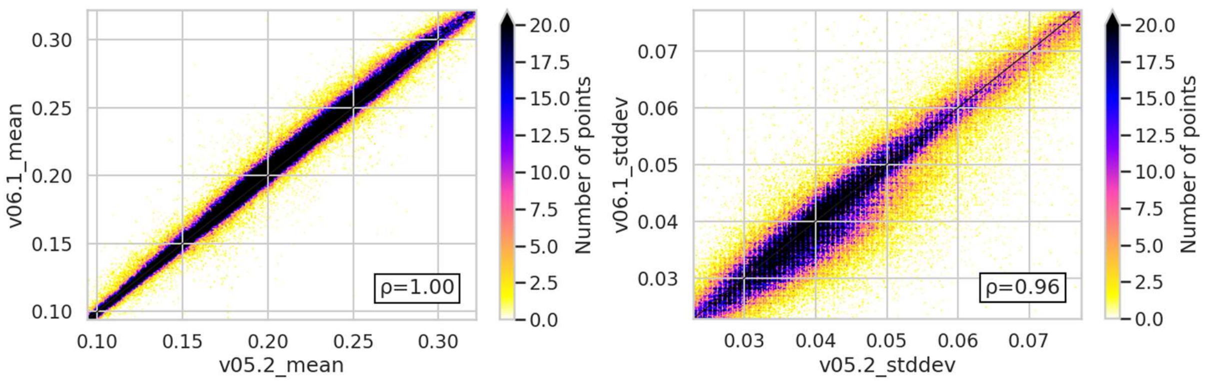

Figure 10: Comparison of the mean (left) and standard deviation (right) of the ESA CCI SM v06.1 and v05.2 COMBINED datasets.

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 analysed.

Figure 11 shows the anomalies for the year 2020 for Europe for the ESA CCI SM v06.1 COMBINED product. The same is shown in Figure 12 for the v05.3 COMBINED product (Note: v05.3 is used here as it is the temporally extended version of v05.2 and therefore can be used to compare anomalies from 2020).

There are a few small differences in the global anomaly plots between the dataset versions. ESA CCI SM v06.1 provides drier anomalies in some areas (for example northern Africa) but wetter anomalies in other areas (for example the eastern USA). It appears that the newer dataset results in more extreme anomalies (both wetter and drying) implying that the mean for the reference period (1991-2010) may have a lower variance than in v05.3 which is partially supported by the standard deviation comparison shown in Figure 10 (right).

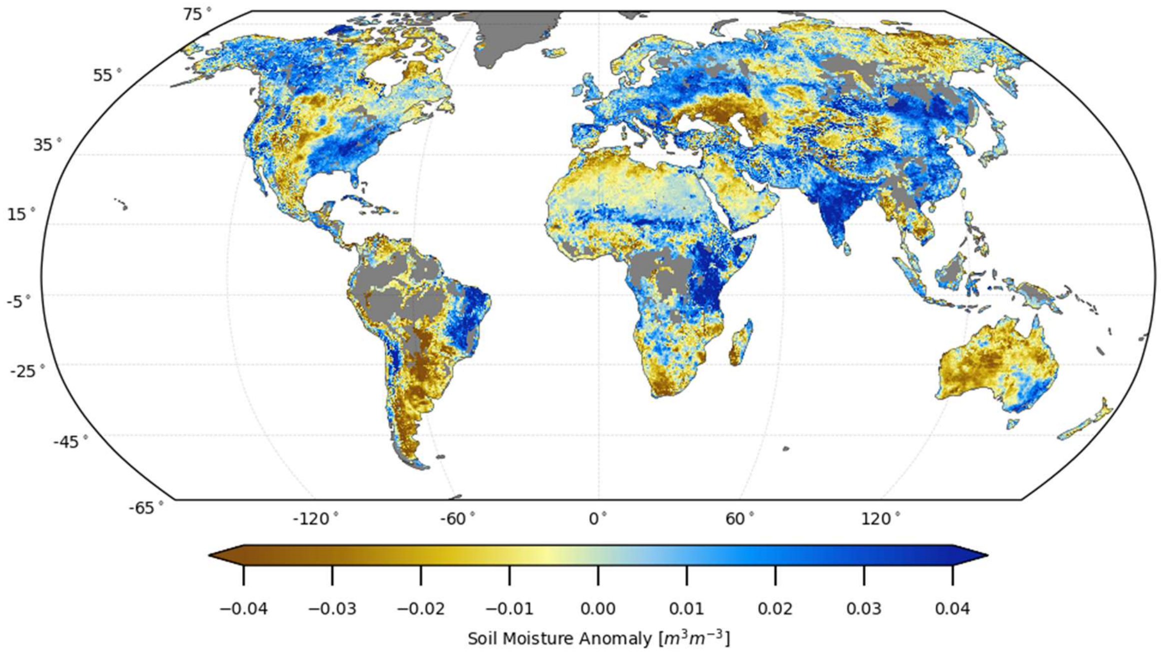

Figure 11: Soil moisture anomalies for the year 2020 from the ESA CCI SM v06.1 COMBINED product (reference period 1991-2010).

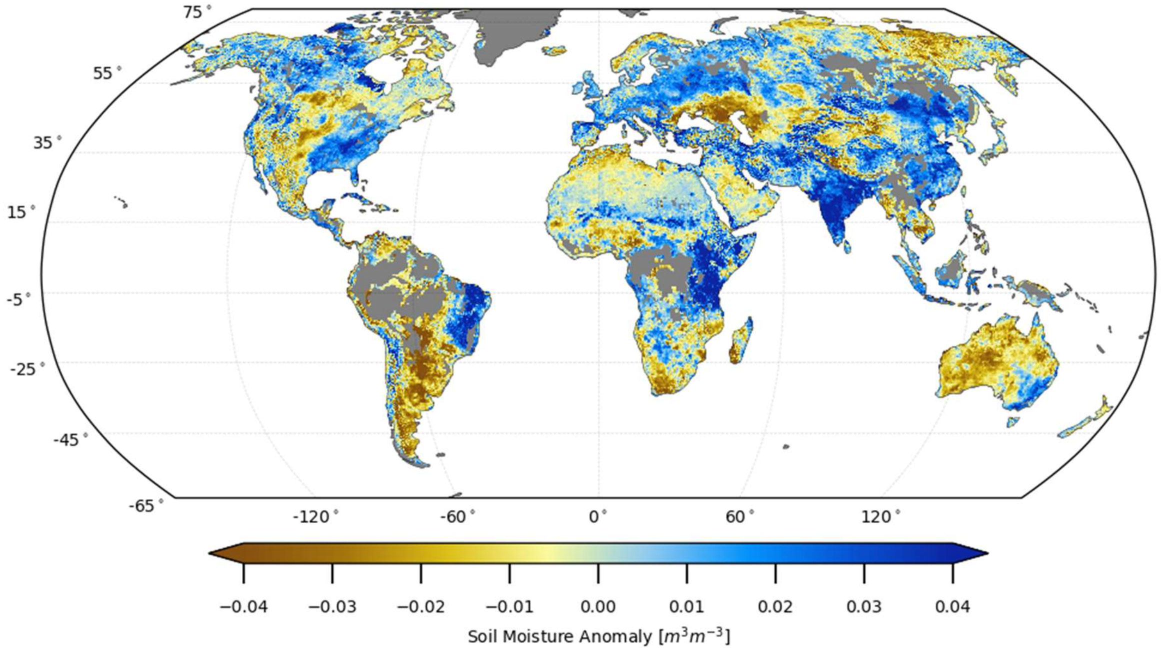

Figure 12: Soil moisture anomalies for the year 2020 from the ESA CCI SM v05.3 COMBINED product (reference period 1991-2010).

5.1.6 Basic Validation against ERA5 Soil Moisture

Validation of ESA CCI SM v06.1 COMBINED against ERA5 soil moisture has been undertaken using the QA4SM framework (www.qa4sm.eu) run locally to allow the inclusion of v06.1. An inter-comparison (i.e., common observations only) was undertaken using v06.1 COMBINED, v05.2 COMBINED and ERA5 soil moisture for the period 2007-01-01 to 2019-12-31.

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 v06.1 affect this period. This means that that the validation results provide clearer information about how the product has changed between v05.2 and v06.1.

Mean – standard deviation scaling has been undertaken to reduce systematic biases between the dataset prior to validation and spatial matching is undertaken using nearest neighbour (CCI is matched to the nearest ERA5 point and results are presented on the ERA5 grid). Temporal matching is also undertaken using nearest neighbour (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 v06.1 COMBINED is shown in Figure 13. The generally expected spatial patterns of correlation are seen, with good agreement shown in most areas. Lower correlations are shown primarily in northern latitudes and in areas of bare soils.

Figure 14 shows the difference in correlation with ERA 5 between v06.1 and v05.2. The areas shown in blue represent improvements in the correlation with the new dataset. The major improvements are in northern latitudes where the improved snow flagging has been implemented. There is a reduction in performance against ERA 5 in over some parts of China and the source of this degradation will be investigated in future CCI versions.

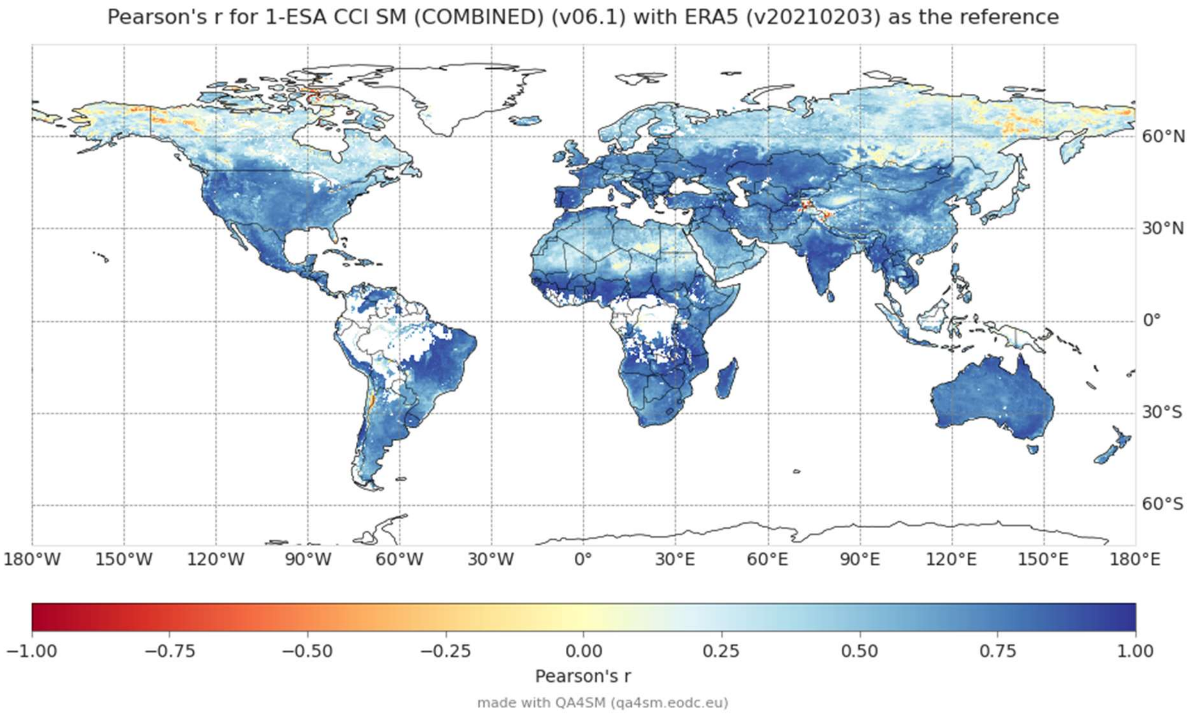

Figure 13: Pearson's correlation between ESA CCI SM v06.1 COMBINED and ERA5 soil moisture for the period 2007-01-01 to 2019-12-31.

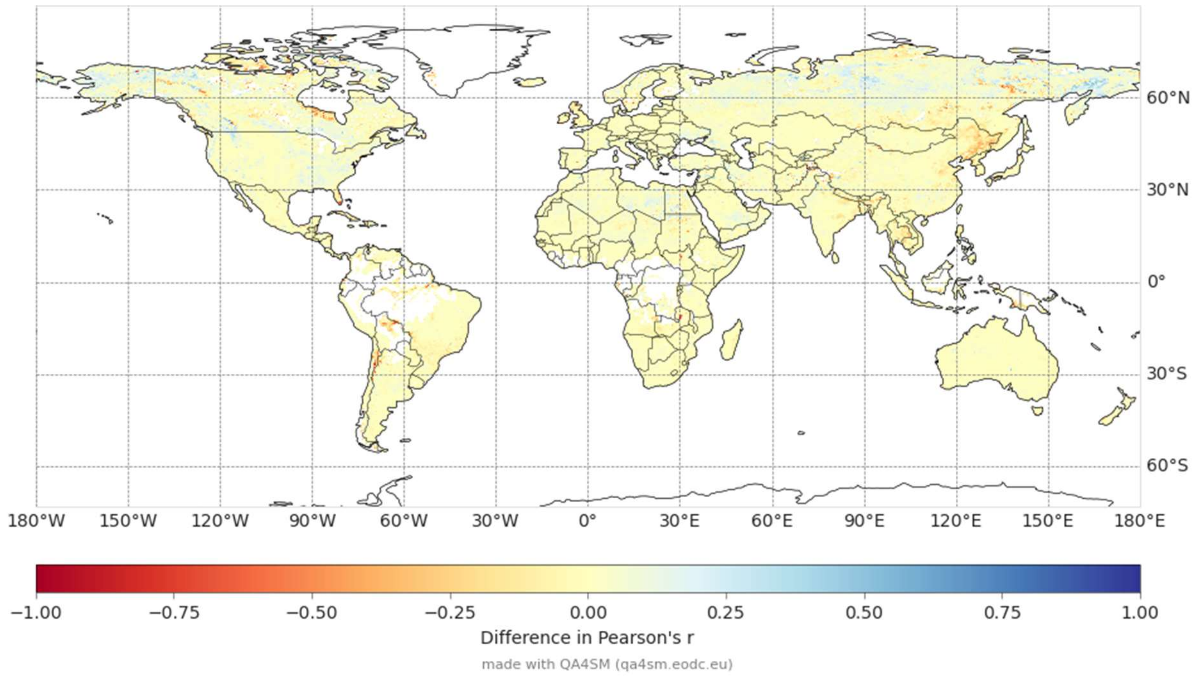

Figure 14: Difference in Pearson's correlation against ERA5 soil moisture between ESA CCI SM v06.1 COMBINED and v05.3 COMBINED for the period 2007-01-01 to 2019-12-31.

5.1.7 Break-Adjusted COMBINED Product

At v06.1 a new experimental product is provided in addition to the main ESA CCI SM product. This break-adjusted COMBINED product is produced using the methodology set out in [*Preimesberger et al.*, 2021; also described briefly in the ATBD [RD-02]].

The basic quality checks for data completeness have also been applied to this dataset and the coverage is the same as those shown for the COMBINED product in Figure 1 and Figure 3, which is as expected. No uncertainty field is provided with the break-adjusted product as the method for estimating how uncertainties change through the break correction procedure has not yet been developed.

The difference Hovmöeller diagram, with the original product subtracted from the break-adjusted product, is shown in Figure 15. The largest effect is in the Southern hemisphere in the period 2002 to 2011 (i.e. the AMSR-E period) where the break adjusted product provides lower values than the original product. In the northern hemisphere differences can be seen prior to 2002 where the break adjusted product provides higher values than the original product. These differences can also be seen in the monthly averaged time series (Figure 16).

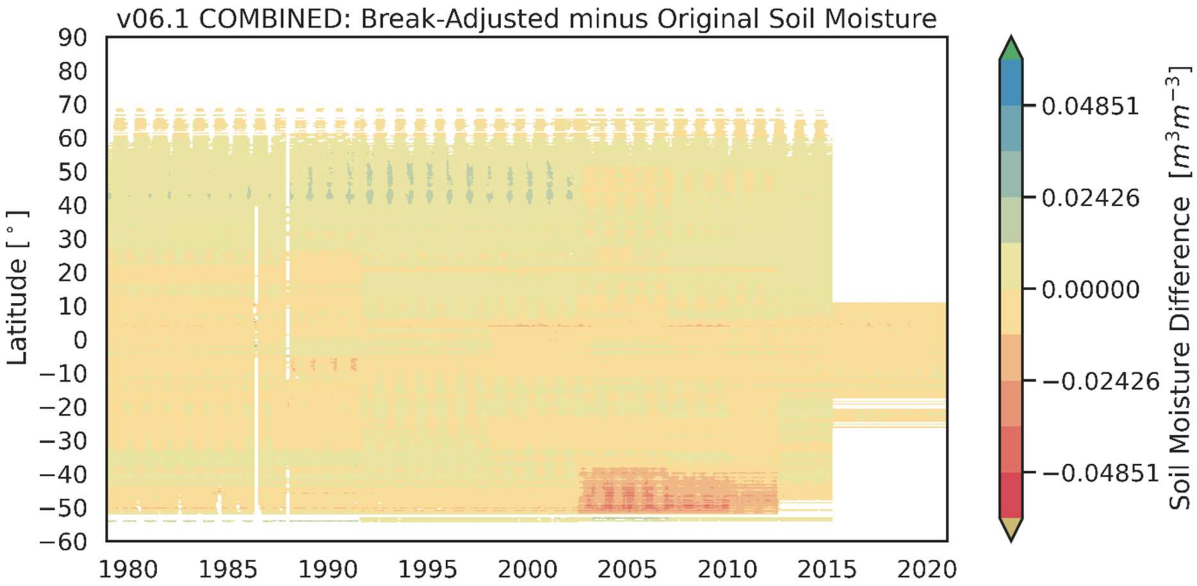

Figure 15: Differences in soil moisture Hovmöeller for the ESA CI SM v06.1 COMBINED break-adjusted product vs. the original, non-break-adjusted original ESA CCI SM v06.1 COMBINED product. Soil moisture is averaged per month and per latitude. Note: areas of high vegetation are masked out from the monthly / latitude aggregation. Red (negative) means that the break-adjusted product provides lower soil moisture values than the original product.

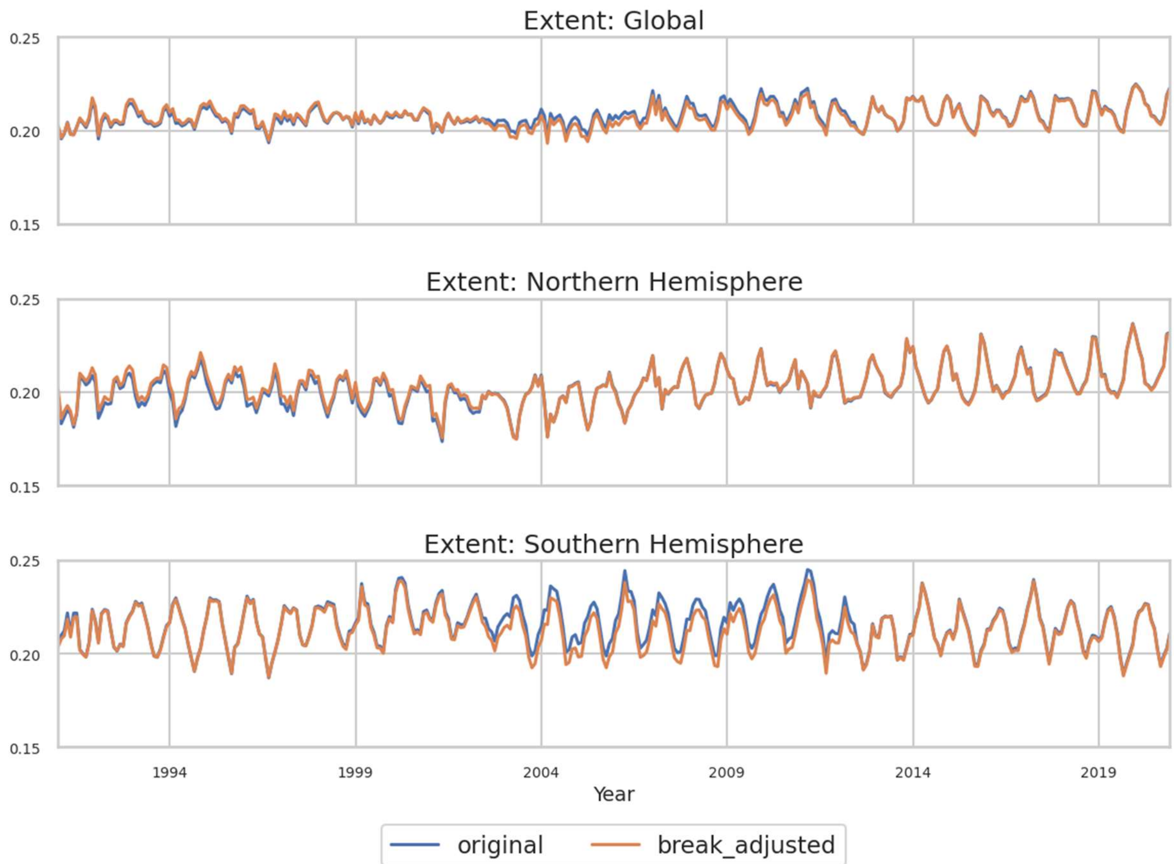

Figure 16: Comparison of the monthly averaged time-series for the original ESA CCI SM v06.1 COMBINED product and the break-adjusted product.

5.1.8 Summary

The following points summarise the conclusions of the above sections:

- The ESA CCI SM v06.1 product provides spatial and temporal coverage in line with previous versions with additional observations available due to the inclusion of GPM, FY-3B and the extension of TMI.
- The uncertainty provided with the ESA CCI SM v06.1 product are complete.
- The general statistics of the data are, as expected, and in line with previous versions, with a slight reduction in the standard deviation of some spatial points for ESA CCI SM v06.1 COMBINED compared to v05.2.
- The soil moisture anomalies in v06.1 COMBINED are in line with previous versions however, for 2020, some areas show more extreme anomalies than previous version.
- There are some improvements between the new v06.1 dataset and v05.2 dataset when compared to ERA 5. These improvements are primarily in the northern latitudes and align with the new snow flagging implemented in the input datasets.
- The break-adjusted product provides primarily changes the soil moisture time series in two distinct periods mainly at extreme latitudes.

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

5.2.1 Datasets and data processing

<u>ESA CCI SM</u>

To date various versions of the ESA CCI SM product are available. We use here v0.1, v02.2, v03.3, v04.7, v05.2 and the newest v06.1 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 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 v06.1 and v05.2 are used for some of the analyses, as well as a break-adjusted version of the v06.1 COMBINED product [*Preimesberger et al.*, 2021]. 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].

<u>ISMN</u>

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.*, 2011]. The analyses are based on a full download from 11 February

2021. 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, ERA-Interim/Land, MERRA-2

To determine the influence of soil depth on soil moisture variability, we use ECMWF's ERA5-Land reanalysis soil moisture [*C3S*, 2019]. 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. Moreover, the forerunner of ERA5-Land, ERA-Interim/Land [*Balsamo et al.*, 2015; *Dee et al.*, 2011] is used for comparison and as previous reanalysis benchmark in some of the analyses. For the analysis of the long-term temporal trends, also surface soil moisture of the atmospheric reanalysis MERRA-2 is included [*Gelaro et al.*, 2017].

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 17) as well as the time period 1991-2010 when considering all major ESA CCI SM product releases. This selection results in 311 individual soil moisture time series from 18 different networks. Soil moisture time series from the grid cells in which the stations fall are extracted from ESA CCI SM, ERA5-Land and ERA-Interim/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). This, depending on the temporal subset under investigation, considers the extended set of currently available ISMN data with up to 700 stations.

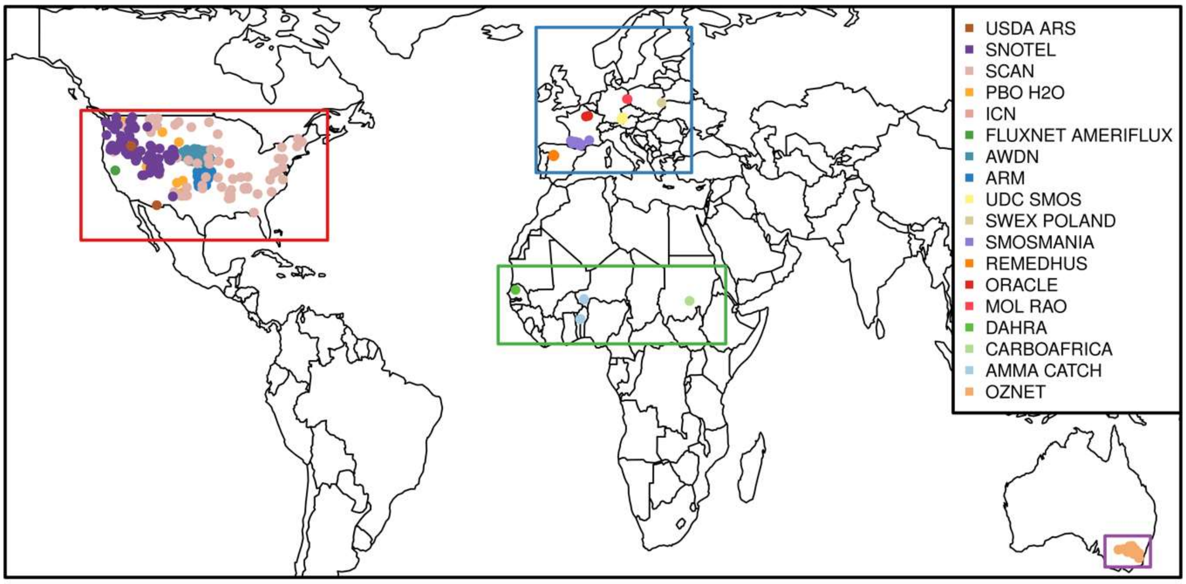

Figure 17: Overview of the spatial coverage of the stations considered in this section, rectangles indicate the four focus areas of the comparison, i.e., the United States (US, red), Europe (EU, blue), Africa (AF, green), and Australia (AUS, purple). Stations are color coded by network, see Figure 18 for the legend.

Comparisons of the products

We focus on the evaluation of ESA CCI SM v06.1 COMBINED and compare it to its forerunners v0.1, v02.2, v03.3, v04.7 and v05.2 as well as to ERA5-Land and ERA-Interim/Land layer 1 and layer 2 soil moisture. Additionally, the ACTIVE and PASSIVE products of v06.1 and v05.2 are use 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 18).

To account for the different units and dynamic ranges of the products, and to remove systematic differences between the products, the ESA CCI SM, ERA5-Land and ERA-Interim/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, ERA5-Land and ERA-Interim/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.

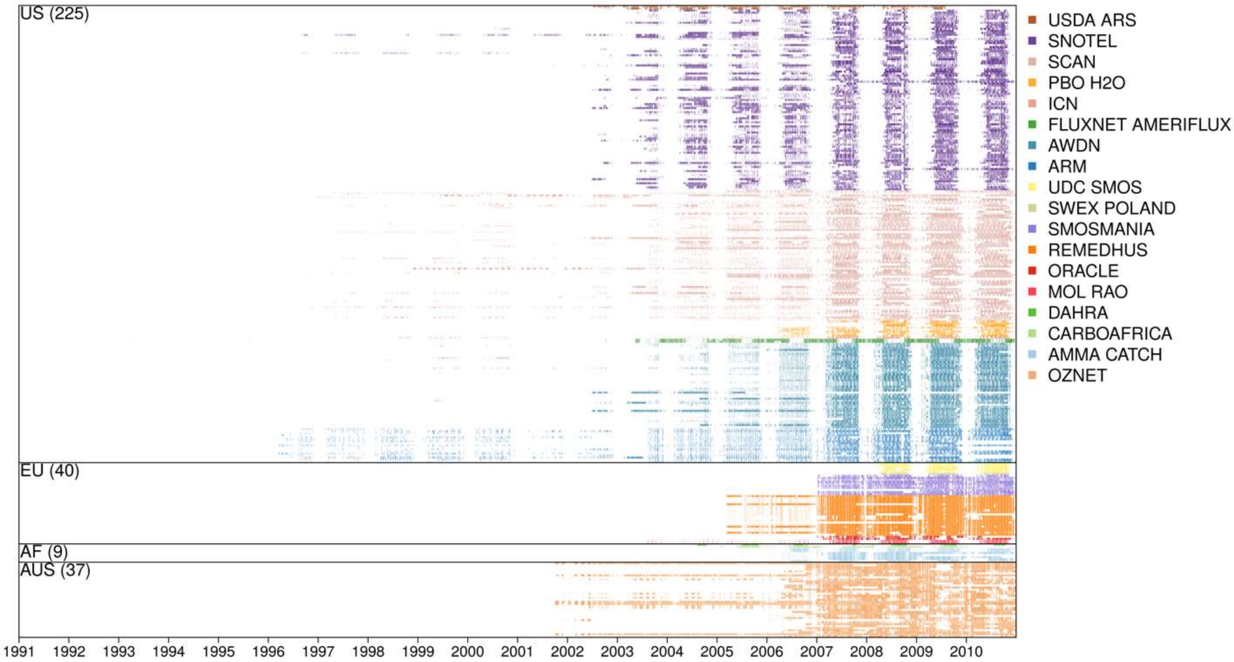

Figure 18: Overview of the temporal coverage of the stations considered in this section, after masking for common data availability, split per region. The number of stations per region is indicated in brackets.

5.2.2 General findings

Figure 19 shows the distribution of the correlation and ubRMSD values from the comparison of ESA CCI SM v05.2 and v06.1 (COMBINED, ACTIVE, PASSIVE) with respect to the full set of ISMN stations (i.e., up to 700 stations, 5 cm measuring depth) over the common 1992-2019 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.

A tendency for higher correlations can be observed for v06.1 for the absolute soil moisture values. Such an increase in the skill between v05.2 and v06.1 is less clearly visible for ubRMSD as well as for the inter-annual anomalies (based on the confidence intervals of the median estimates, Table 2 and Table 3). 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.

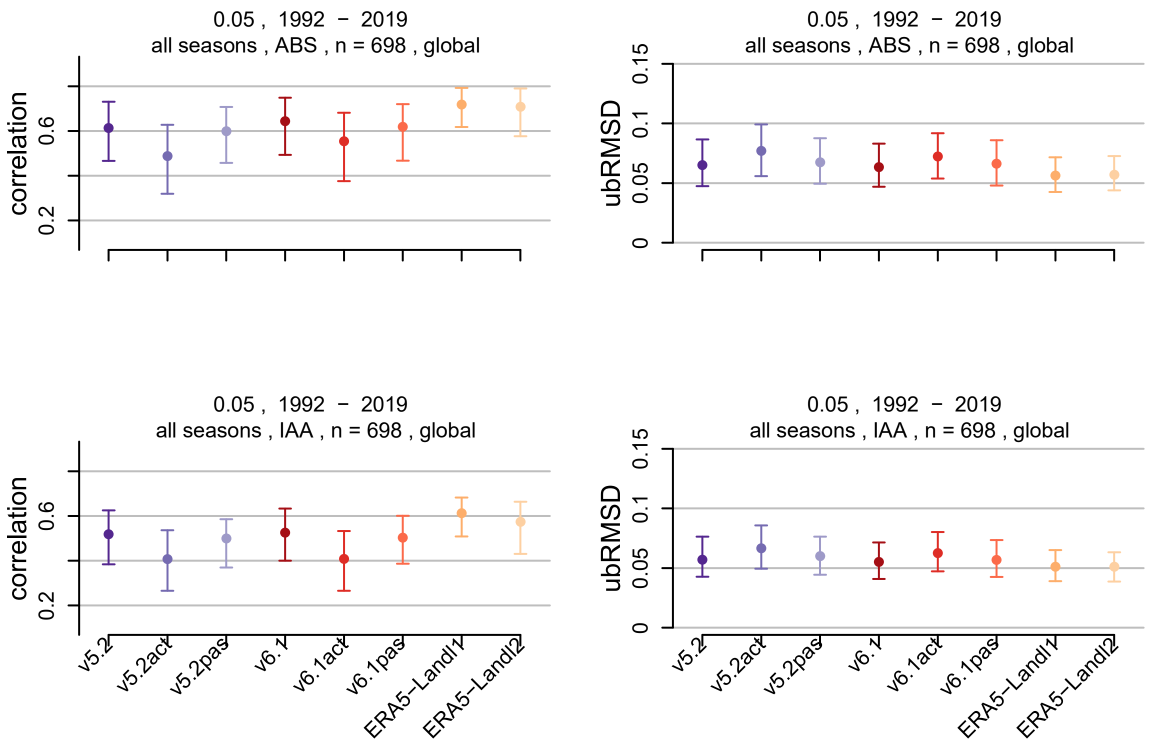

Figure 19: Correlation (left) and ubRMSD (right) of the last two releases of ESA CCI SM (v05.2 and v06.1 COMBINED, ACTIVE and PASSIVE; the latter two denoted as vX.Yact and vX.Ypas) as well as of ERA5-Land (layers 1 and 2)) as compared to the full set of ISMN in-situ station observations (5 cm measurement 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 v05.2 and v06.1 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	
	v05.2	v06.1	v05.2	v06.1	v05.2	v06.1
Correlation [-]	0.613 [0.583;0.636]	0.644 [0.625;0.664]	0.487 [0.470;0.510]	0.554 [0.526;0.576]	0.599 [0.581;0.620]	0.618 [0.598;0.636]
ubRMSD [m^3/m^3]	0.065 [0.062;0.068]	0.063 [0.061;0.066]	0.077 [0.074;0.079]	0.072 [0.070;0.075]	0.068 [0.064;0.070]	0.066 [0.064;0.069]

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

Metric	COMBINED		ACTIVE		PASSIVE	
	v05.2	v06.1	v05.2	v06.1	v05.2	v06.1
Correlation [-]	0.518 [0.503;0.535]	0.525 [0.509;0.540]	0.407 [0.390;0.423]	0.408 [0.387;0.427]	0.499 [0.490;0.520]	0.503 [0.487;0.518]
ubRMSD [m³/m³]	0.057 [0.054;0.059]	0.055 [0.053;0.057]	0.067 [0.064;0.069]	0.063 [0.060;0.065]	0.060 [0.058;0.063]	0.057 [0.055;0.058]

For different climate zones (Figure 20 and Figure 21), the correlations and ubRMSDs also indicate better agreement of ERA-Interim/Land and in particular of ERA5-Land with the in-situ data compared to different ESA CCI SM COMBINED releases, i.e., considering the first public version of the product (v0.1) and the respective major releases of the main product generations [as represented by the evolution of the merging algorithm; see *Gruber et al.*, 2019]. The skill of ESA CCI SM appears to be slightly better for arid climate zones, both for absolute values and anomalies. A slight increasing tendency in the skill is visible for the subsequent major ESA CCI SM releases.

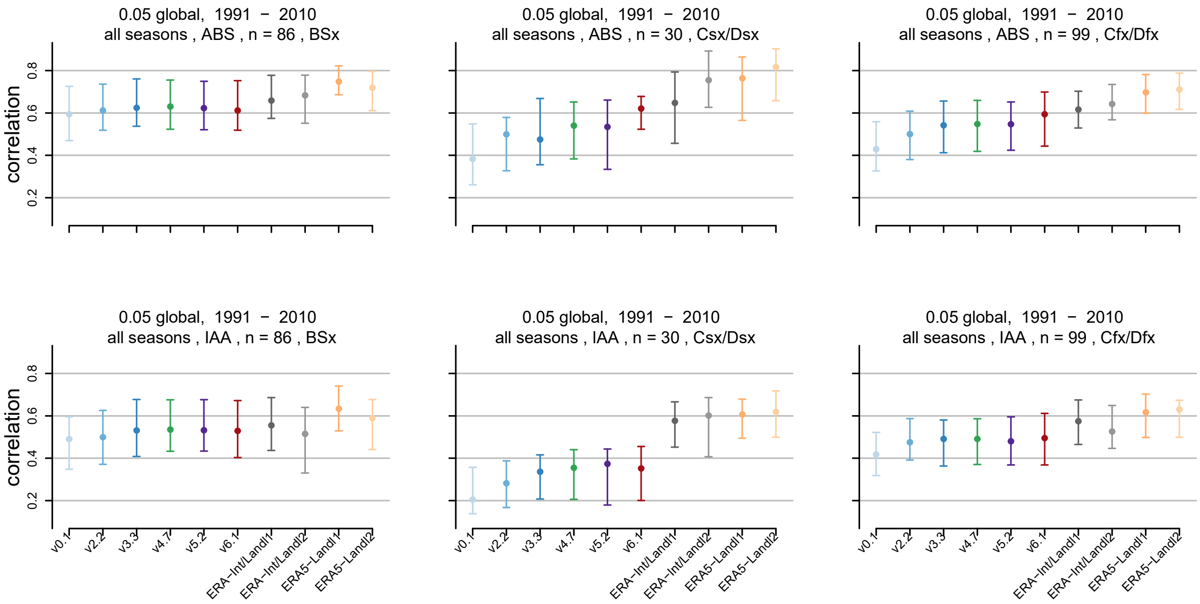

Figure 20: Correlation of the gridded soil moisture products (ESA CCI SM v0.1, v02.2, v03.3, v04.7, v05.2 and v06.1 COMBINED, as well as ERA-Interim/Land and ERA5-Land (layers 1 and 2)) as compared to in-situ station observations (5 cm depth) for three combinations of Köppen-Geiger classes (BSx - arid, 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.

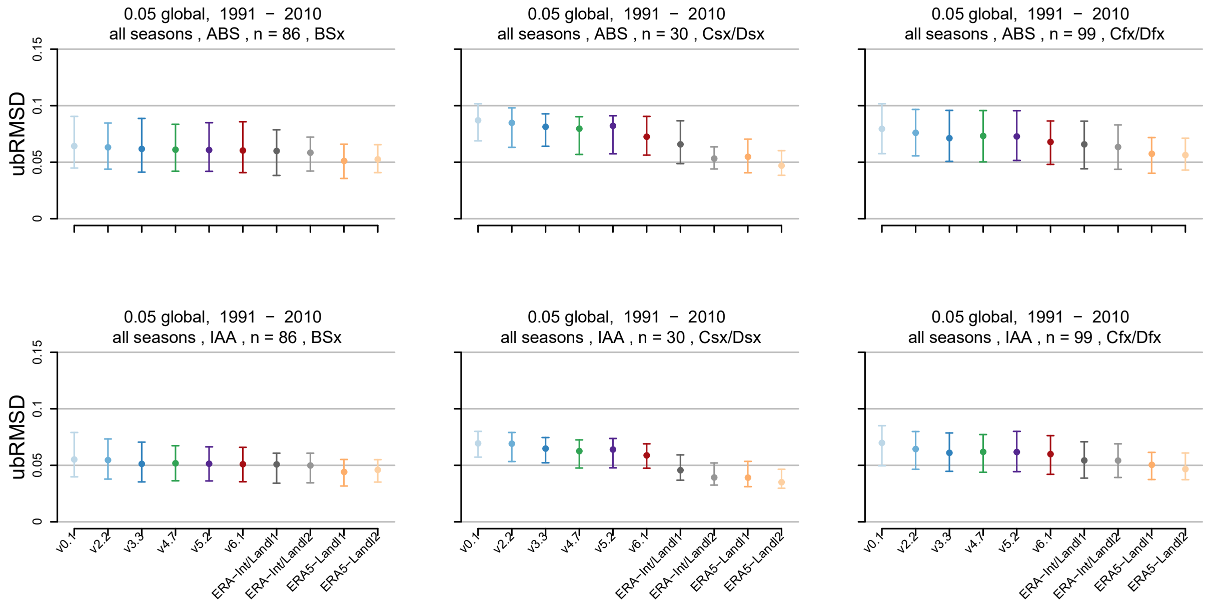

Figure 21: As Figure 20, but showing ubRMSD.

Focusing on the US only where spatial coverage with in-situ stations is most dense (Figure 22), 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. Also, no pronounced difference in performance can be found between networks (not shown). 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 v0.1 to v06.1. ERA5-Land layer 1 shows better agreement with in-situ soil moisture than ESA CCI SM, for both absolute values and anomalies.

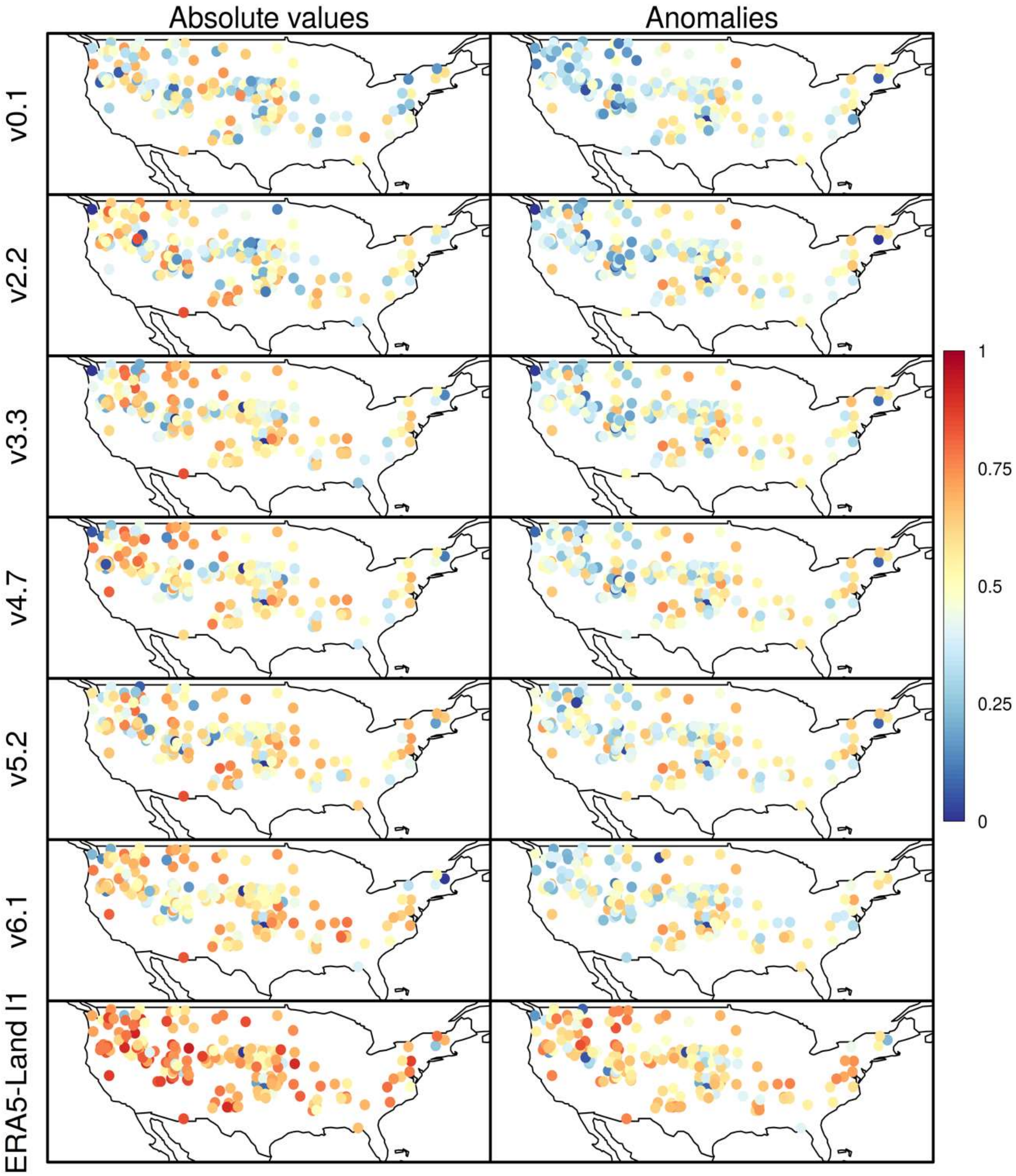

Figure 22: Correlation between in-situ soil moisture and ESA CCI SM for versions v0.1, v02.2, v03.3, v04.7, v05.2 and v06.1 COMBINED, as well as ERA5-Land soil moisture layer 1 (ERA5-Land l1, 0-7 cm), for absolute soil moisture (left) and the anomalies (right) and the period 1991-2010.

5.2.3 Temporal subsets and product evolution

Figure 23 shows the (significantly positive, $p < 0.05$) correlations of the different ESA CCI SM releases, as well as ERA5-Land and ERA-Interim/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., 1997-2000, 2001-2004, 2005-2008, 2009-2012, 2013-2016 and 2017-2020, as well as 1997 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 2001-2004 and subsequent increase towards later periods. This behaviour is in particular visible for summer (not shown). The correlations of ERA5-Land are more stable over time, while ERA-Interim/Land also displays a drop in 2001-2004. 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 the periods after 2000 and is also visible in clear improvements from v05.2 to v06.1 for these later time slices. As for the global validation with ISMN, the PASSIVE and ACTIVE products of v06.1 show lower skill compared to the COMBINED product.

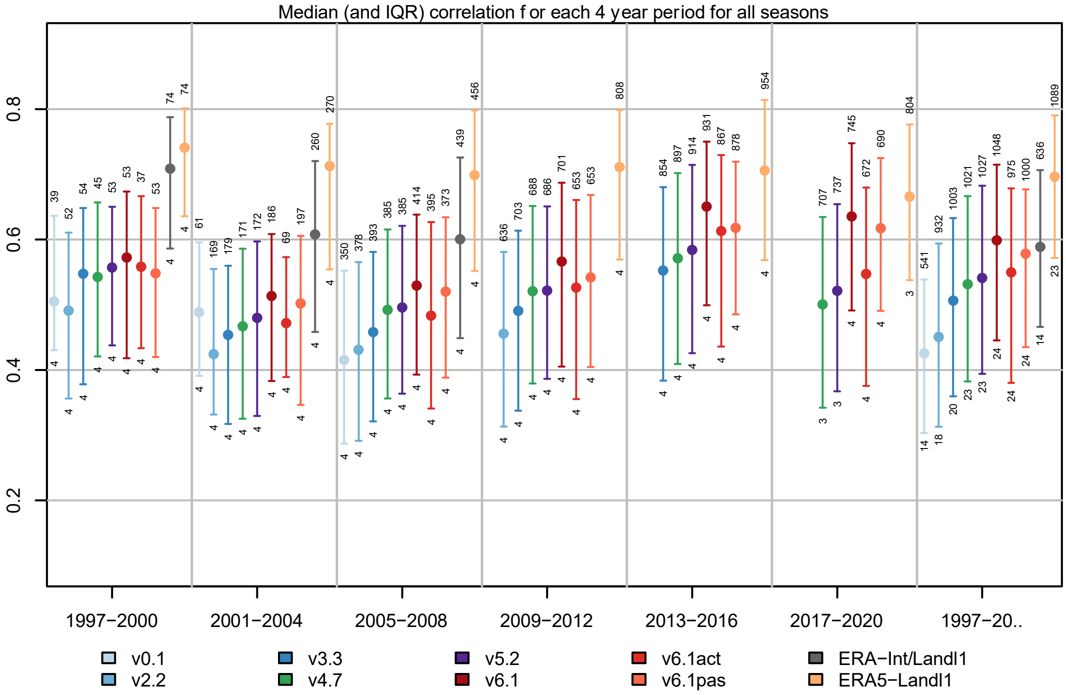

Figure 23: Correlation of the gridded soil moisture products as compared to in-situ station observations in 5 and 10 cm depth for the full year for the US. Subdivided in consecutive 4-year periods (1997-2000, 2001-2004, 2005-2008, 2009-2012, 2013-2016 and 2017-2020) as well as for the longest period data is available (1997-20.., end date would e.g. be 2010 for CCI v0.1, but is 2020 for e.g. CCI v06.1). 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 releases of ESA CCI SM COMBINED, the ACTIVE and PASSIVE products are also shown in case of v06.1 (denoted v6.1act and v6.1pas).

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 measurements at 5 and 10 cm depth, see Figure 24.

As noted above, the near-surface measurements may be more prone to errors [*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 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) as well as the anomalies (bottom). 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 0.8 for the comparison with the 5 cm in-situ measurements, and between 0.1 to over 0.6 for the 10 cm measurements, with the median correlation for the shallower 5 cm in-situ measurements being consistently higher. For Europe, the correlations are higher with a median value over 0.6 for 5 cm depth for ESA CCI SM v0.1, and over 0.7 for v06.1. Again, the correlation with in-situ measurements at 10 cm depth is lower, though there are also less measurements available at this depth. The overall highest correlations are found in Australia, with up to 0.8 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 appears less pronounced, in particular in the US (where v0.1 even shows a reversed behavior, i.e., slightly higher 10 cm median correlation).

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 correlation is less dependent of the measuring depth, both for absolute values and the anomalies. For ERA5-Land l2, correlation with measurements taken at 10 cm are slightly higher in this region. For the anomalies, the results are comparable, though here the median correlation for 10 cm is also higher over Europe for ERA5-Land l2. The range of the correlations is similar to ESA CCI SM but goes 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.

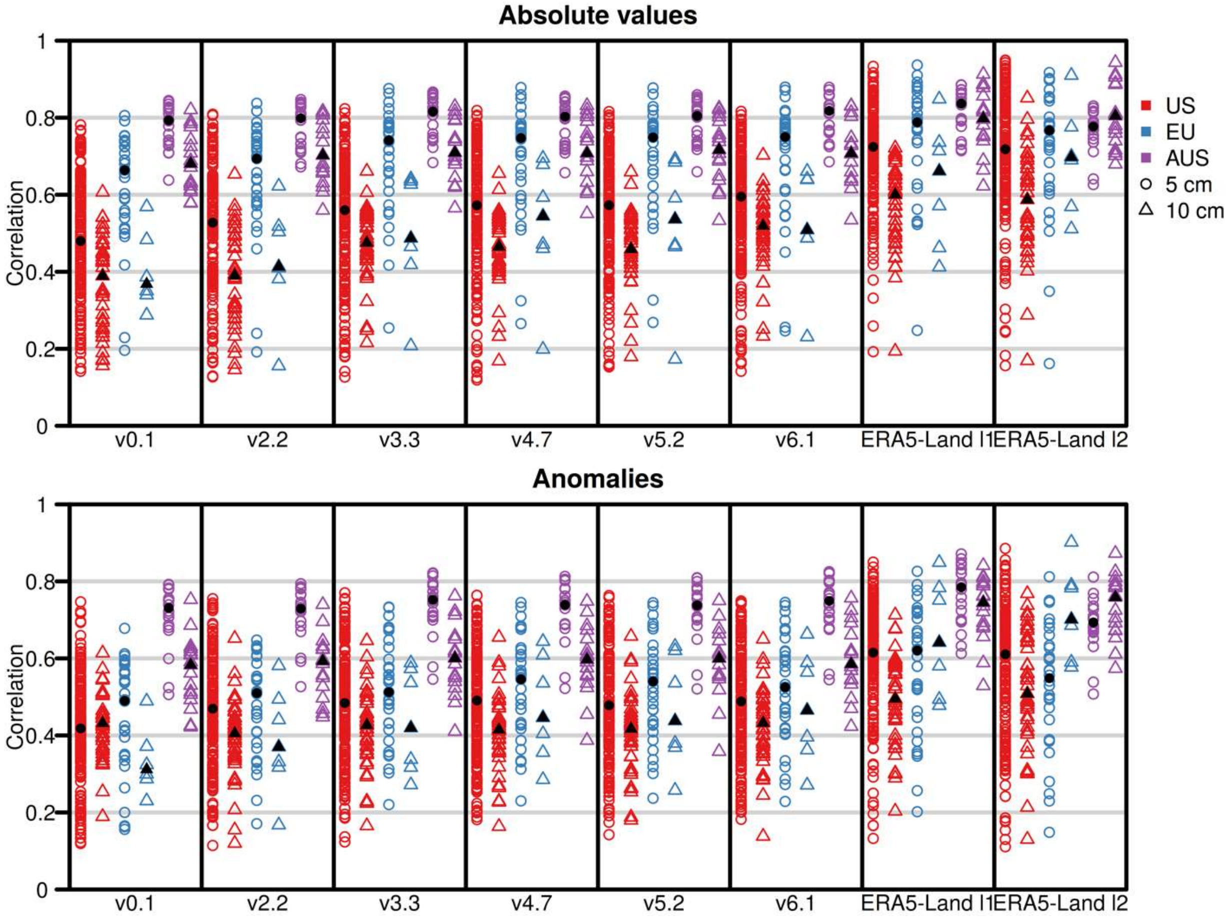

Figure 24: Correlation between in-situ measurements and ESA CCI SM v0.1, v02.2, v03.3, v04.7, v05.2 and v06.1, as well as ERA5-Land soil moisture layer 1 and 2 for the absolute soil moisture values (top) and the anomalies (bottom). For each product, we distinguish between 3 regions US, EU, and AUS (red, blue and purple, AF has insufficient data coverage), and the correlation at 5 cm depth (circles) and 10 cm depth (triangles) over the 1991-2010 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 25 shows the correlations of ESA CCI SM v0.1, v02.2, v03.3, v04.7, v05.2 and v06.1 (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 all versions of ESA CCI SM, there is 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 not visible.

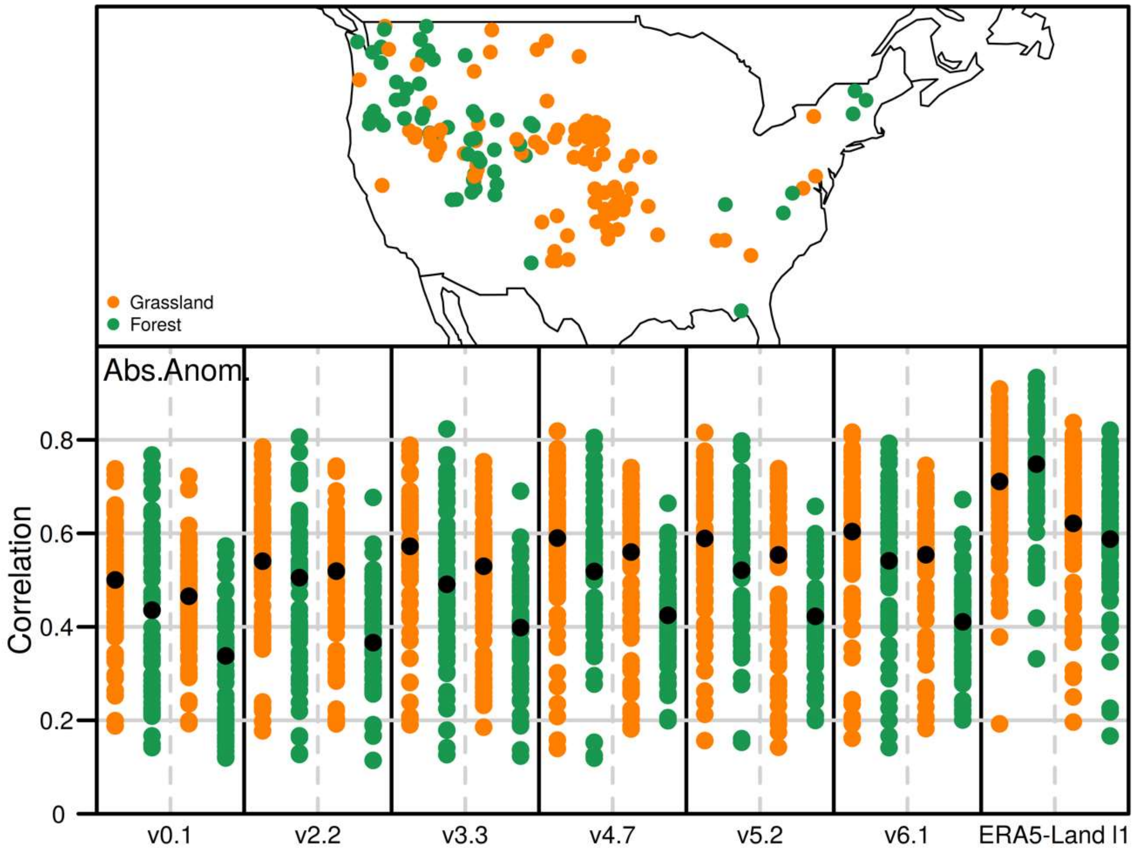

Figure 25: Correlation between in-situ measurements at 5 cm depth and ESA CCI SM v0.1, v02.2, v03.3, v04.7, v05.2 and v06.1, as well as ERA5-Land soil moisture layer 1 over the 1991-2010 time period, differentiating between grassland (orange) and forest (green) sites for absolute soil moisture values 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, which corresponds to overall higher correlations and lower ubRMSDs in arid climate.
- ESA CCI SM clearly shows a higher correlation with in-situ measurements at 5 cm depth than at 10 cm depth. For ERA5-Land this distinction is less clear.
- Also, ESA CCI SM clearly shows higher correlations with in-situ measurements over grassland sites than over forest sites. For ERA5-Land this difference is not visible.
- In particular 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, pointing to the increasing maturity of the remote sensing product. Also, ESA CCI SM v06.1 shows a clear improvement over v05.2 for more recent time periods.

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, the 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 the break-adjusted version of ESA CCI SM v06.1 COMBINED is included in this analysis [*Preimesberger et al.*, 2021]. Theil-Sen trend estimates for the 1988-2010, 1992-2019 and 2007-2019 time periods are presented (Figure 26 - Figure 28), and significance is determined using Mann-Kendall trend tests (p-value < 0.05 for significant trends).

5.3.2 Results

Significant trends in the different product versions (COMBINED products of ESA CCI SM v0.1, v02.2, v03.3, v04.7, v05.2 and v06.1) are only partly consistent (Figure 26). In particular, a large-scale tendency for more widespread positive trends in the northern mid-latitudes is visible with later product versions. Also, the original significant wetting trend in southern Africa disappears with the latest product releases, while Patagonia starts to experience wetting trends.

Comparing the last two product releases of ESA CCI SM (v06.1 and v05.2, COMBINED products), significant trends appear more similar, however ESA CCI SM v06.1 shows less widespread negative trends in the high latitudes (true for all considered time periods). Similarly, the significant negative trends in the ACTIVE product disappear in Siberia from v05.2 to v06.1 (Figure 27 and Figure 28). The break-adjusted product of v06.1 displays very similar trend patterns compared to the non-adjusted version for all considered time periods.

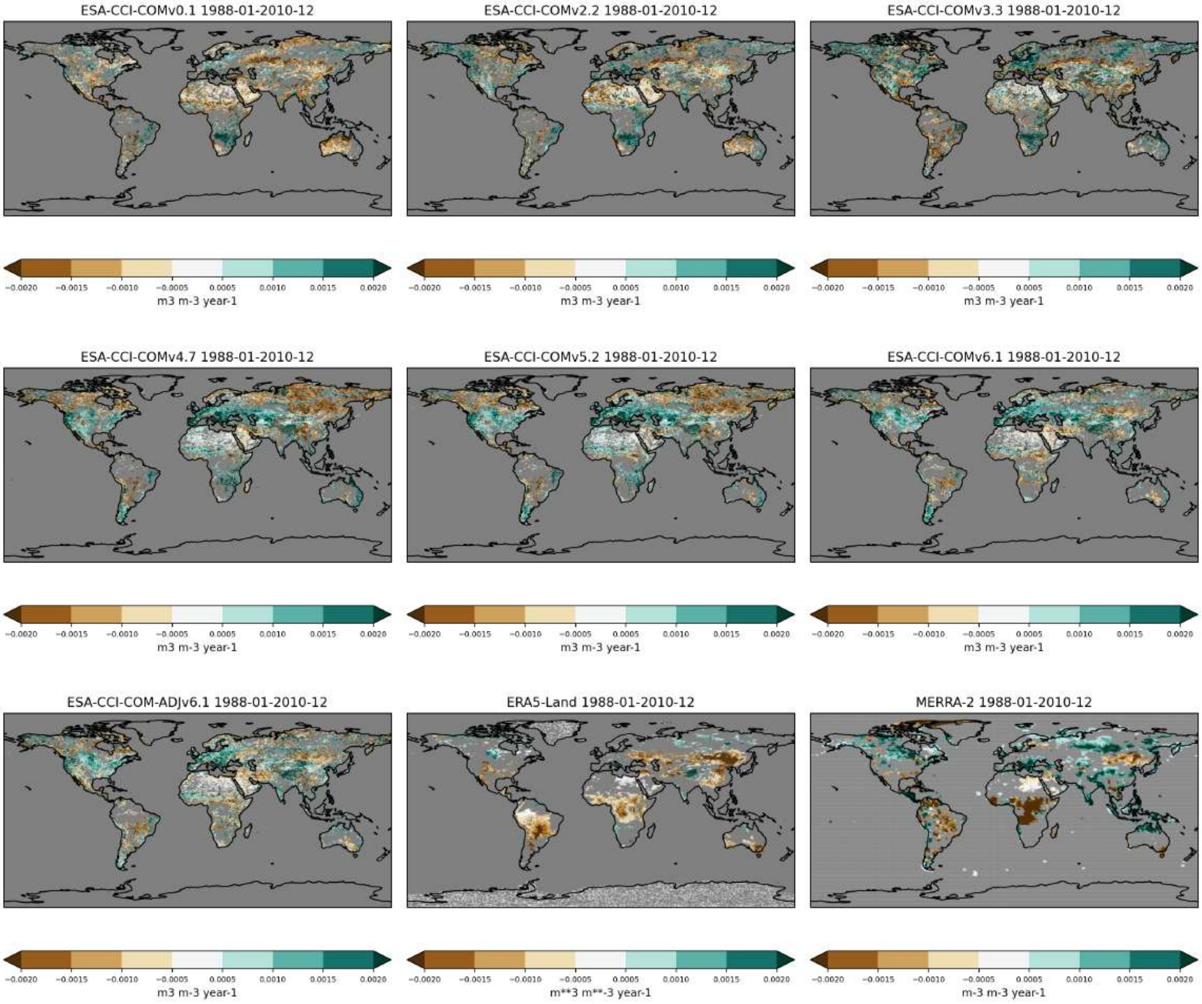

Figure 26: Evolution of 1988-2010 trends with the major product releases ESA CCI SM (v0.1, v02.2, v03.3, v04.7, v05.2 and v06.1 COMBINED products, as well as break-adjusted version of v06.1), and in comparison to ERA5-Land and MERRA-2. Theil-sen trend estimate based on yearly mean surface soil moisture ($m^3 m^{-3}$ 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 trend signals of ESA CCI SM v06.1 COMBINED, and the ERA5-Land and MERRA-2 reanalysis products are also diverse and only partly consistent. In particular, ERA5-Land shows predominantly negative trends for the 1988-2010 and 1992-2019 time periods, while MERRA-2 and ESA CCI SM v06.1 COMBINED show larger fractions of positive trends (Figure 26 and Figure 27). Differences in the distribution of significant trends over the 1992-2019 time period are also visible between the COMBINED, ACTIVE and PASSIVE products of both ESA CCI SM v06.1 and v05.2. In particular, the PASSIVE products display widespread negative trends in Europe, western USA and central Asia, while the COMBINED and ACTIVE products display no significant or positive trends in these regions (Figure 27). On the other hand, the significant positive 1992-2019 trends in southern Africa appear more widespread in the PASSIVE product. For recent 2007-2019 trends, the different ESA CCI SM products appear to be slightly more consistent.

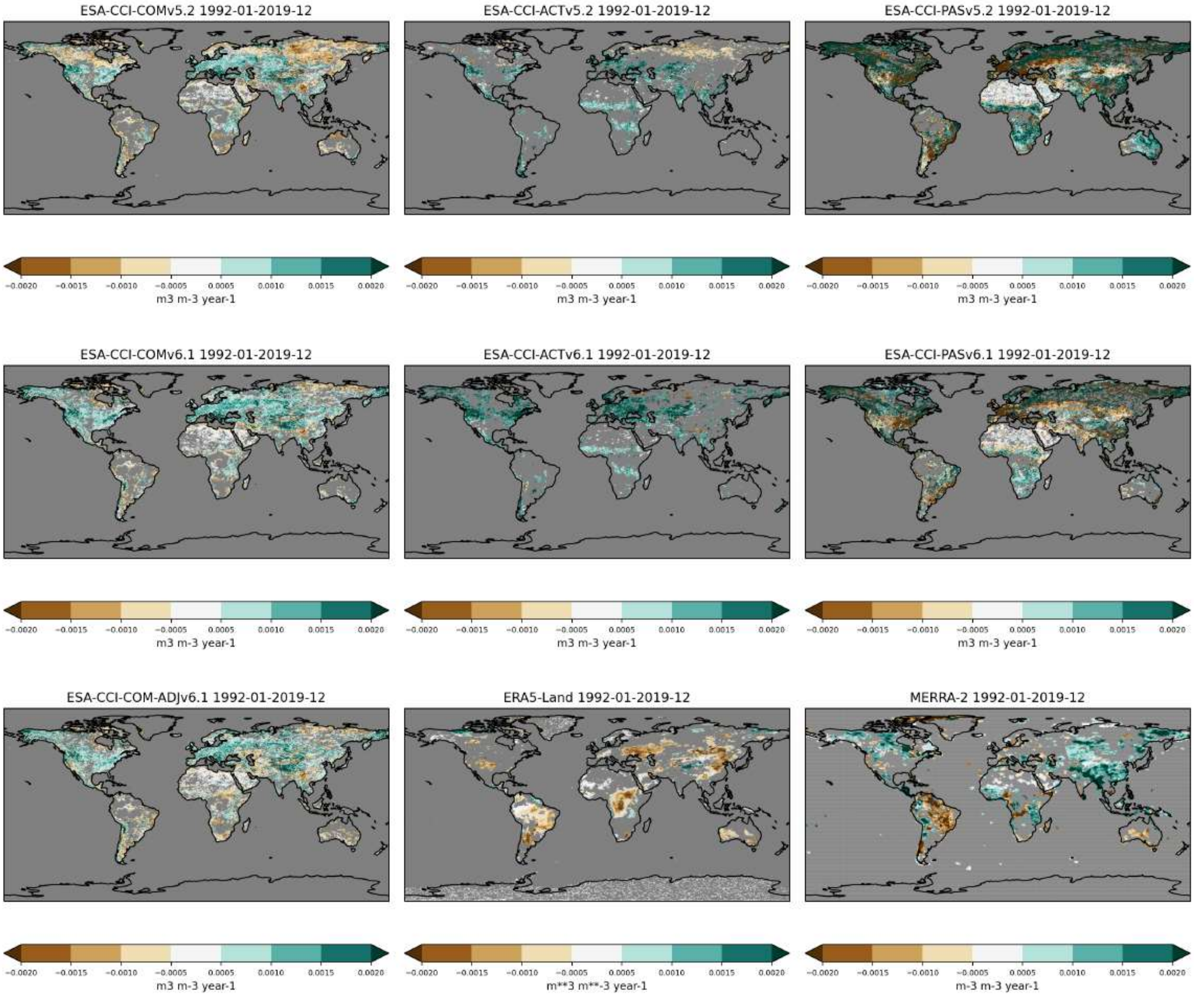

Figure 27: As Figure 26, but for the long-term 1992-2019 trends of v06.1 and v05.2 COMBINED, ACTIVE and PASSIVE, as well as the break-adjusted product of v06.1, and in comparison to ERA5-Land and MERRA-2.

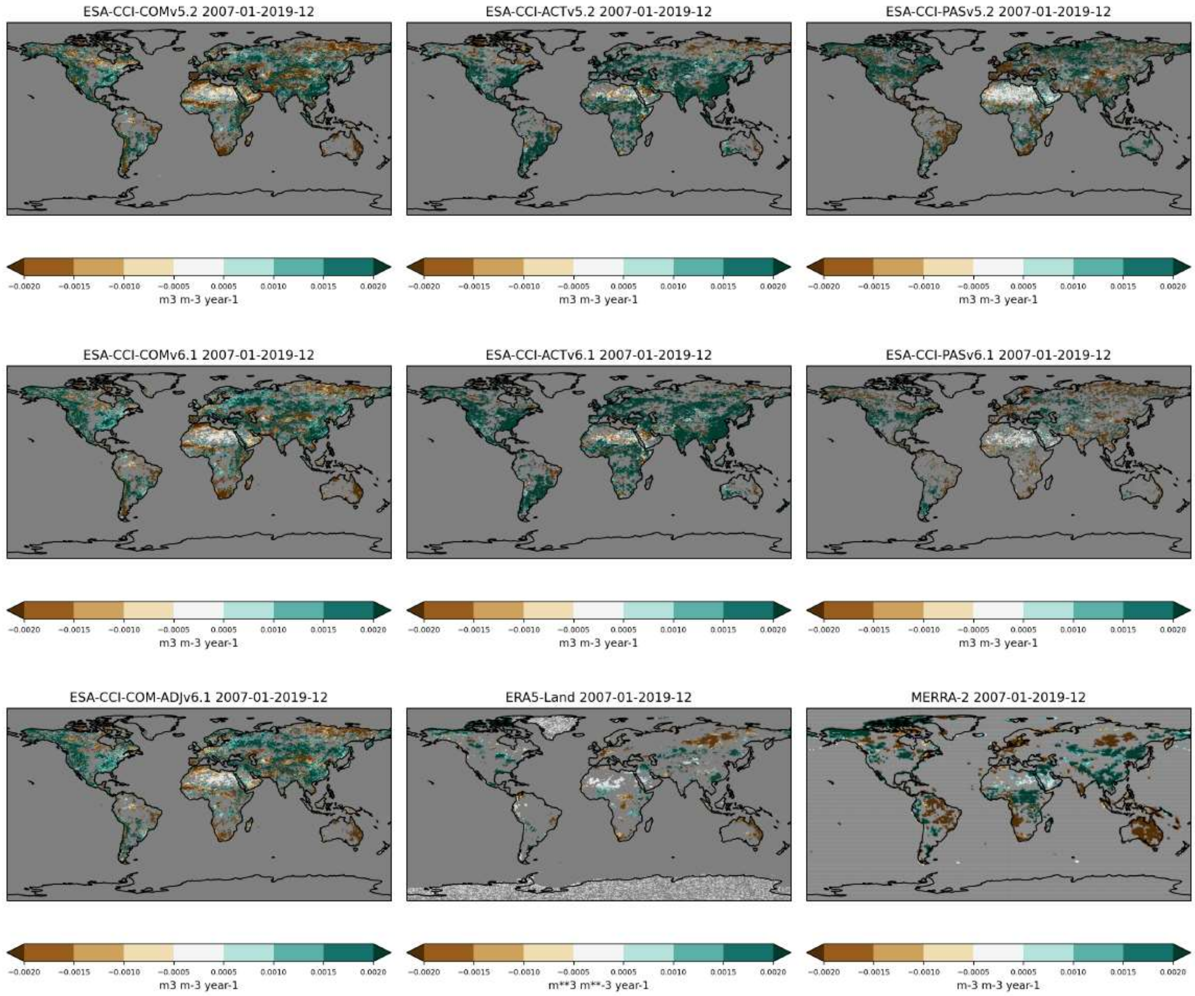

Figure 28: Figure 27, but for the recent 2007-2019 trends.

5.3.3 Summary

- The representation of long-term significant trends over the common 1988-2010 time period shows changes with the evolution of ESA CCI SM (COMBINED product).
- Significant trend patterns partly diverge between the ESA CCI SM COMBINED, and the underlying ACTIVE and PASSIVE products, as well as compared to reanalysis products.
- Trends in the last two product releases of ESA CCI SM COMBINED (v06.1 vs. v05.2) appear more similar, though v06.1 shows less widespread negative trends in the high latitudes.

6 Conclusions

Based on the various verification and validation activities described in this PVIR, the current ESA CCI SM v06.1 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 product shows a general increase in skill with subsequent major data releases, which points to the increasing maturity of the ESA CCI SM product.

The agreement of ESA CCI SM with in-situ measurements appears slightly better for arid climate. Moreover, previous validation activities further showed that the ESA CCI SM product suffers shortcomings at northern high latitudes (northward of 60°N, though improving from earlier products), over regions with complex topography and regions with dense vegetation, all areas well known to be difficult to monitor from remote sensing platforms.

Within the ESA CCI SM v06.1, 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.

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 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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