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Soil Moisture ECV Product User Guide (PUG) Revision 3 D3.3.1 Version 4.5

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Prepared by

Earth Observation Data Centre for Water Resources Monitoring (EODC) GmbH



in cooperation with

TU Wien, VanderSat, CESBIO and ETH Zürich



ETH zürich



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For any clarifications please contact Richard Kidd (richard.kidd@geo.tuwien.ac.at).



Project Partners	
Prime Contractor and project management	EODC, Earth Observation Data Centre for Water Resources Monitoring (Austria)
Earth Observation Partners	TU Wien, Vienna University of Technology (Austria) VanderSat, The Netherlands CESBIO, France
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Definitions, acronyms and abbreviations

Acronym	Full Name			
AMI-WS	Active Microwave Instrument - Windscat (ERS-1 & 2)			
AMSR-E	Advanced Microwave Scanning Radiometer-Earth Observing System			
ASCAT	Advanced Scatterometer (Metop)			
ATBD	Algorithm Theoretical Basis Document			
CCI	Climate Change Initiative			
CECR	Comprehensive Error Characterization Report			
DARD	Data Access Requirement Document			
DMSP	Defense Meteorological Satellite Program			
DPM	Data Processing Model			
EASE	Equal-Area Scalable Earth			
ECV	Essential Climate Variable			
ERA-				
Interim	ECMWF Reanalysis Interim			
ERA-Land	ECMWF Reanalysis land water resources dataset			
ERS	European Remote Sensing Satellite (ESA)			
ESA	European Space Agency			
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites			
FTP	File Transfer Protocol			
GCOS	Global Climate Observing System			
GLDAS	Global Land Data Assimilation System			
IODD	Input Output Data Description			
ISEA	Icosahedron Snyder Equal Area			
ISEA4H	Icosahedron Snyder Equal Area (ISEA) Aperture 4 Hexagonal			
JAXA	Dokuritsu-gyosei-hojin Uchu Koku Kenkyu Kaihatsu Kiko, (Japan Aerospace Exploration Agency)			
JULES	Joint UK Land Environment Simulator			
LDAS	Land Data Assimilation System			
MERRA	Modern-Era Retrospective Analysis for Research and Applications			
ΜΕΤΟΡ	Meteorological Operational Satellite (EUMETSAT)			
MIRAS	Microwave Imaging Radiometer using Aperture Synthesis			
NaN	Not A Number			
NASA	National Aeronautics and Space Administration			



- NWP Numerical Weather Prediction
- PDF Probability Distribution Function
- PSD Product Specification Document
- PUG Product User Guide
- SAR Synthetic Aperture Radar
- SM Soil Moisture
- SMMR Scanning Multichannel Microwave Radiometer
- **SMOS** Soil Moisture and Ocean Salinity
- SRD System Requirements Document
- SSD System Specification Document
- SSM Surface Soil Moisture
- SSM/I Special Sensor Microwave Imager
- SURFEX SURFace EXternalized module
- SWI Soil Water Index
- TBD to be determined
- TMI TRMM Microwave Imager
- TRMM Tropical Rainfall Measuring Mission
- UTC Coordinated Universal Time



1 Executive Summary

The ESA CCI SM v04.5 product consists of three surface soil moisture data sets: The "ACTIVE Product" and the "PASSIVE Product" were created by fusing scatterometer and radiometer soil moisture products, respectively; The "COMBINED Product" is a blended product based on the former two data sets. Data files are provided as NetCDF-4 classic format and comprise global merged surface soil moisture datasets at daily temporal resolution. The data set spans over 40 years covering the period from November 1978 to December 31st 2018.

The theoretical and algorithmic base of the product is described in [RD-3], and reported by Wagner et al. (2012). The SNR (signal-to-noise-ratio) merging algorithm introduced for the first time in version 3.2 is described in Gruber et al. (2017). An overview of all known errors of the soil moisture datasets is provided in Gruber et al. (2017) and in (Gruber et al. 2017). Further documentation relating to the product, and reference documents are provided in Section 3 and can be found on the CCI Soil Moisture project web site (<u>http://www.esa-soilmoisture-cci.org</u>).

The location and full access details to the product are provided to users after completion and verification of a user registration form. Users can register to access the product from the User Registration form on the CCI Soil Moisture Website.

The product is provided in a format that currently complies with the minimum standard format requirements as detailed by the CCI data standards working group (DSWG) [RD-11]. For this reason ESA CCI SM v04.5 is provided in NetCDF-4 classic format and is also compliant with the NetCDF Climate and Forecasting group best practice¹ [RD-12].

¹http://cf-pcmdi.llnl.gov/documents/cf-conventions/latest-cf-conventions-document-1



2 Introduction

2.1 Purpose and structure of the Document

The purpose of the Product User Guide (PUG) is to describe the ECV data product in a manner that is understood by the product user with focus on:

- the geophysical data product content
- the product flags and metadata
- the data format
- the product grid and geographic projection
- how people use the product and the tools available, and
- known limitations of the product.

Since the users of the soil moisture product come from a wide and varied audience, with differing levels of knowledge in the field of retrieval of soil moisture information from satellite observations, this document provides some relevant background aiming to enable a common understanding. Section 4 provides an overview of the pivotal role that soil moisture plays within the environment and section 5 provides an overview of its retrieval from earth observation satellites.

In section 6 the product characteristics are introduced including the geophysical parameters that are available in the products, their respective data volumes, and the physical structure and format of the product and associated quality flags and indicators.

Section 7 is largely taken from (Gruber et al. 2017) and it presents the broadest review, to date, of the current use and application of the ESA CCI SM product by the wider scientific community. In this section it is shown how ESA CCI SM has contributed to improved process understanding in the following Earth system domains: climate variability and change, land-atmosphere interactions, global biogeochemical cycles, hydrological and land surface modelling, drought applications, and meteorology. The exhaustive list of references for this section are presented in Section 12.

Known issues and product limitations, for the data producers point of view, are provided in Section 8 and picks up on such points as the spatial availability of the data and provides information on the fraction of days with valid observations over the different periods of the data set and show fractional observation density across the globe. In Section 9 the opportunity is taken to provide an overview of key points relating to data access, team contact, and restates the acknowledgement to be cited in the use of the ECV SM products. Reflecting on the broad and varied backgrounds of the users Section 10 concludes the PUG with the provision of some common terminology used within the earth observation domain.



2.2 Target Audience

This document targets users of remotely sensed soil moisture data sets across the various user domains.

3 Reference Documents

The following references are of relevance to this document.

[RD-1]	ESA Climate Change Initiative Plus, Statement of Work, European Space Agency, ESA_CCI-EOPS-PRGM-SOW-18-0118.
[RD-2]	Technical Proposal (Part 3) in response to ESA Climate Change Initiative Plus AO/1-9322.18/I-NB , Vienna University of Technology.
[RD-3]	ATBD, Algorithm Theoretical Baseline Document, D2.1 Version 04.5, Executive Summary 2nd October 2019, ESA Climate Change Initiative Plus Soil Moisture Project, http://www.esa-soilmoisture-cci.org
[RD-4]	M. Ertl, A. Boresch,(2013) System Specification Document (SSD v2), Version 2.0, 06 December 2013
[RD-5]	R. Kidd, D. Chung, W. Dorigo, R. De Jeu, (2013) Input/Output Data Definition Document (IODD v2), Version 2.0, 19 December 2013
[RD-6]	CECR, Comprehensive Error Characterisation Report, Version 0.5, 21 April 2015, ESA Climate Change Initiative Phase 2 Soil Moisture Project, http://www.esa- soilmoisture- cci.org/sites/default/files/documents/public/Deliverables/CCI2_Soil_Moisture _D2.2.0_CECR_v0.6.pdf
[RD-7]	DARD, Data Access Requirements Document, Version 4.4, 11th November 2018, ESA Climate Change Initiative Phase 2 Soil Moisture Project, http://www.esa- soilmoisture- cci.org/sites/default/files/documents/public/Deliverables/CCI2_Soil_Moisture _D1.3.0_DARD_v04.4.pdf
[RD-8]	SRD, System Requirements Document, Version 2.0, 9th June 2015, ESA Climate Change Initiative Phase 2 Soil Moisture Project
[RD-9]	R. Kidd, D. Chung, W. Dorigo, R. De Jeu, (2013), Detailed Processing Model (DPM), Version 2.2, 18 December 2013
[RD-10]	PSD, Product Specification Document, Version 4.5, 2 October 2019, ESA Climate Change Initiative Plus Soil Moisture Project



[RD-11]	ESA, Guidelines for Data Producers - Climate Change Initiative Phase 1, CCI- PRGM-EOPS-TN-13-0009, Issue 1, Revision 1, Victoria Bennett and Sarah James, 24/05/2013
[RD-12]	NetCDF Climate and Forecast (CF) Metadata Conventions: Version 1.7, 10 August 2017, Brian Eaton, Jonathan Gregory, Bob Drach, Karl Taylor, Steve Hankin, Jon Blower, John Caron, Rich Signell, Phil Bentley, Greg Rappa, Heinke Höck, Alison Pamment, Martin Juckes, Martin Raspaud



4 Soil Moisture within the environment

The central role of soil moisture for the environment is well known. Its contribution e.g. to hydrological and agricultural processes, linked to e.g. runoff generation, drought development, and irrigation, respectively, is evident. Moreover, it significantly impacts the climate system through feedbacks to the atmosphere. As a source of water for evapotranspiration over the continents, soil moisture is involved not only in the water but also in the energy cycle. Approximately 60% of precipitation over land is returned to the atmosphere as evapotranspiration (Oki and Kanae 2006), and this flux also uses up more than 50% of all net radiation over land (Dirmeyer et al. 2006). The investigations of possible effects of soil moisture on the climate date back to the 70s and 80s (Shukla and Mintz 1982). In the recent years soil moisture-climate interactions received an increasing attention (Seneviratne et al. 2010). Moreover, in 2004 soil moisture was recognised as an essential climate variable (ECV) and finally added in 2010 to the list of terrestrial ECV by the Global Climate Observation System (GCOS).

A number of numerical experiments have established the sensitivity of atmospheric fields to soil moisture dynamics (Diffenbaugh et al. 2007; Fischer et al. 2007a; Jaeger and Seneviratne 2011; Koster et al. 2004a; Seneviratne et al. 2006b). On short time scales, which are relevant for numerical weather prediction, soil moisture variations seem to have a more significant influence on the surface energy budget and on the planetary boundary layer structure than changes in other terrestrial variables such as roughness or albedo (Mahfouf 1991). The importance of soil moisture for sub-seasonal and seasonal forecasting is also well established (Koster et al. 2004a; Koster et al. 2010), and is additionally impacted by the memory associated with soil moisture (Entin et al. 2000; Seneviratne et al. 2006b; Vinnikov et al. 1996; Wu and Dickinson 2004).

Most of the impacts of soil moisture on the climate system are induced by its coupling to evapotranspiration, and resulting impacts on temperature and precipitation (Seneviratne et al. 2010). Strongest feedbacks between land and atmosphere are expected in regions with soil moisture-limited evapotranspiration regimes, given by the control of soil moisture on evapotranspiration (Hirschi et al. 2011). Mostly affected are transitional zones located between wet and dry climates (Koster et al. 2004a; Seneviratne et al. 2006b), where soil moisture is limiting for evapotranspiration and can strongly vary on both intra-annual and inter-annual time scales. This coupling has been shown to be of strong relevance for climate variability in mid-latitude regions, in particular for the occurrence of heat waves (Fischer et al. 2007c). Impacts on precipitation are less consistent across studies, but are found to include a number of direct and indirect feedbacks (Findell and Eltahir 2003). In the context of climate change, regions with transitional climate regimes are expected to be shifted polewards, with a possible increase in climate variability induced by soil moisture feedbacks in regions with currently wet climate regimes. Supporting numerical studies, recent observational studies



have shown evidence for soil moisture impacts on hot extremes (Hirschi et al. 2011) as well as global evapotranspiration (Jung et al. 2010).

Furthermore, it is possible that soil moisture anomalies may also affect large-scale circulation patterns. For the United States, the study of Pal and Eltahir (2003) has suggested that soil moisture anomalies over relatively small regions may induce floods and droughts not only locally, but also over distant areas. A relationship between the depletion of early summer soil moisture and the development of heat lows over the Mediterranean region in late summer has also been noticed in Haarmsa et al. (2009).

A factor influencing soil moisture-climate interaction is the vegetation. Transpiration is the evaporation through the plant stomata, which is regulated by several factors including soil moisture. Therefore, land cover and its variation in time are expected to play a crucial role for soil moisture-climate interactions. A possible impact of vegetation cover during the European heat wave 2003 was shown in Zaitchik et al. (2006) by comparing temperature anomalies over pastures and forests, showing higher heat anomalies over the pastures during the August peak of the 2003 European summer drought and heat wave. The study by Teuling et al. (2010), based on measurements from the Fluxnet network, also identified differences in the energy fluxes over grassland and forest sites during heat wave days, although the results were in partial contrast to those of Zaitchick et al. (2006). For typical heat wave days, it was found that the forest led to a higher warming of the atmosphere than grassland, because the former used less energy for evapotranspiration than the latter. However, the implications are that in the long term the soil moisture depletion over grassland is faster than over forest, and consequently grassland would lead to higher warming after long dry and hot periods. This study highlighted the time-scale dependence of feedbacks between land surface processes and the climate, and its strong relation to soil moisture dynamics.

All of the mentioned feedbacks and interactions are particularly relevant for drought development, and especially agricultural (or soil moisture) drought. This is another area where the increasing availability of soil moisture observations can help investigate and diagnose the underlying driving processes, e.g. the respective role of large-scale circulation patterns versus land-atmosphere feedbacks for drought development (Rowell and Jones 2006; Schubert et al. 2004).



5 Soil Moisture Data from Earth Observation Satellites

This section provides a general overview of the different types of data and the methods, technologies and processes employed to generate the Soil Moisture Data Products from the measurement to their application/analysis.

5.1 Microwave Instruments onboard Earth Observation Satellites

There are two principal types of remote sensing, corresponding to the following types of microwave instruments: (a) scatterometers and radars which measure the radar backscattering coefficient σ^0 in physical units [dB] or $[m^2/m^2]$, and (b) radiometers which measure the brightness temperature T_B in physical unit [K]. Instruments in group (a) are called *active* because they use their sown source of electromagnetic energy for the measurement, while the ones in group (b) are referred to as *passive* instruments because they measure energy that is reflected or emitted from the earth surface.

Figure 1 identifies the active (at the bottom) and the passive (at the top) microwave instruments that are used for the production of the Soil Moisture ECV Data Products, their hosting satellites, and their times of operation.

- AMI-WS and ASCAT are (active) C-band scatterometer instruments onboard the ERS and METOP satellites, respectively. Note that AMI-WS is still labelled "SCAT" in the picture, though the former name is nowadays preferred.
 - SMMR, SSM/I, TMI, AMSR-E, AMSR-2, MIRAS and WindSat are (passive) multifrequency radiometer instruments onboard the Nimbus-7, DMSP, TRMM, Aqua, GCOM-W1, SMOS and Coriolis satellites, respectively.

These instruments are characterized by their high suitability for Soil Moisture retrieval and their technological maturity.



Figure 1: Microwave Instruments used for the generation of Soil Moisture ECV Data Products (version 4.5)

The System is designed to allow the integration of new instruments during its operational use phase. In Figure 1, although the Soil Moisture Active Passive (SMAP) and Aquarius missions are not yet considered in the products generated within phase 2 of the project, they are already included to highlight their potential inclusion in the ECV production in the future. SAR data from Envisat and Sentinel-1 will not be directly integrated into the merged ECV products but be used for improved characterisation of errors and sub-pixel heterogeneity of the coarse-scale products.

In a single overpass (one orbit around the Earth) the satellite's instrument observes a wide swath of the land surface of a width somewhere between 500 to 1400 km. Satellite swath data is made of individual nodes (syn. pixels), each node being a measurement of either backscattering coefficient σ^0 (active) or brightness temperature T_B (passive) from an area (footprint) of 10-50 km diameter on the Earth surface.

Figure 2 shows the geometry of the wide swath imaging measurements made by AMI-WS (SCAT) and ASCAT instruments onboard the ERS and METOP satellites. The AMI-WS scatterometer (left part of Figure 2) consists of three antennae producing three beams looking 45° forward, sideways (90°), and 45° backward with respect to the satellite's motion direction along the orbit. The measurements from each beam consist of 19 nodes spaced 25 km apart. As the satellite beams sweep along the Earth surface yielding an approximately



Figure 2: Beams and Wide Swaths of AMI-WS and ASCAT Instruments

500 km wide swath, each node produces its own σ^0 backscatter measurement, integrated over an area around 50 km in diameter. The three measurements originating from the three beams during the single satellite overpass are called triplets.



Figure 3: Wide Swaths and Daily Global Coverage of AMI-WS (left) and ASCAT (right)

The ASCAT scatterometer (right part of Figure 2) is similar but consists of three antennae on either side, producing six beams. The measurements from each beam consists of 21 nodes

spaced 25 km apart (lo-res) or 41 notes spaced 12.5 km apart (hi-res). While the satellite beams sweep along the earth surface a wide swath is observed on either side.

Figure 3 shows the orbits made by a single ERS satellite (left) and a single METOP satellite (right) and the wide swaths captured by AMI-WS and ASCAT instruments, respectively, during one day of observation time. The wide swaths of ASCAT have near-global revisiting times of 2–3 days.

5.2 Data Processing Chain

The payload data received from a satellite passes through a chain of processing which has the following principal steps:

- Level 0: Reconstructing the raw instrument data from a satellite's payload data transmissions received at satellite ground stations, and archiving them at a data centre.
- Level 1: Converting the raw instrument data of a single overpass swath to calibrated measurements (observations) of radar backscattering coefficient σ^0 in [dB] or $[m^2/m^2]$ (in case of active instrument), or brightness temperature T_B in [K] (in case of passive instrument).
- Level 2: Retrieving the Surface Soil Moisture (SSM) geophysical parameter in physical units [%] or [m³/m³] from the calibrated measurements of a single overpass swath.
- Level 3: Generating the consistent and global Soil Moisture ECV Data Products by merging the SSM timeseries acquired from many satellites over many years this is the objective of the system specified herein.
- Level 4: Analysing the lower level data to determine the state or change of state (events, processes) of regional or global climate systems.

The following section provides a brief survey of the different processing levels tailored to Soil Moisture. There is also a fine-grained organization within the levels, in terms of sublevels or product categories, but these are suppressed in the first survey. A full specification of data processing levels is available in IODD [RD-5].

Levels 0-1:

The steps up to Level 1, from the instrument to the calibrated measurement result, follow the principles of measurement as outlined in (JCGM 2008), and (JCGM 2012). Note that a measurement (syn. observation) is not necessarily made with a single antenna, instrument, or even a single satellite. Crucial is that the individual measurement devices contributing to the measurement result are synchronized (with sufficient accuracy in space and time) to the spatial-temporal coherency characteristics of the observed source. Therefore, the calibrated



measurement may be summed from many antennas (e.g. in case of the SMOS MIRAS instrument, which uses aperture synthesis) or even summed from satellites in formation flying. In any case, because the observations made at different orbits do not satisfy the coherency criteria, Level 1 data are observations from a single overpass.

Levels 2-3:

The situation changes for the Levels 2 and 3, which are about the art of estimating values of quantities that cannot be directly measured with remote sensing instruments. The mathematical-physical basis for this process is that there is a functional relation between object parameters X and instrument observables Y. Symbolically, the relation may be written as Y = f(X) (forward model) or X = g(Y) (inversion). It is known that at any time object parameters X and observables Y have definite values. Once sufficient information is obtained from measurements of Y, estimates of X can be determined under certain conditions, if there is sufficient knowledge of a suitable model or inversion. To indicate this radical difference, this process is no longer called measurement but "retrieval".

In the case of the ECV Production System the observed object is an area of the top soil surface layer (of approx. 25x25 km size and < 2 cm thickness), and the retrieved geophysical parameter is Soil Moisture, expressed in the physical unit [%] or $[m^3/m^3]$.

Depending if the measurement was made with an active or a passive microwave instrument, respectively, either a change detection approach or a forward modelling method is utilized. Both methods, like geophysical parameter retrieval in general, require use of additional ancillary data, which can be long-term reference data (historical data, climate data) or model parameters.

Levels 2 and 3 have in common that the retrieved parameters are local state variables: they characterize the state of a local and compact object in space (i.e. a local physical system), at a moment or period in time. They are thus distributions in space (over the land surface in case of Soil Moisture) and time. The difference between Level 2 and 3 is that the parameter retrieved by a process of Level 2 adheres to the locality condition of a single Level 1 measurement, while this condition is relaxed at Level 3. In practice, Level 3 is about merging Level 2 data from different observation times, orbits or instruments.

For full descriptions of the retrieval and merging methods cf. ATBD [RD-3] and (Wagner 2012).

Level 4:

At Level 4 analyses of data from Levels 3, 2 or 1 are performed in order to determine the state or the change of state of specific geo-physical systems of interest, in particular regional and global climate systems. Detection of change of state typically involves statistical analysis methods (e.g. trend analysis) and process model calculations (simulations) using lower level data as input.



Present at all Levels of the data processing chain (but omitted in the discussion so far) are processes to determine measures for the degree of definiteness of the resulting data. At Levels 0 and 1 an adequate measure is the measurement uncertainty as described e.g. in (JCGM 2008), and at Levels 2 and 3 the error characterization as described in CECR [RD-6]. We do not know what measures are used at Level 4 but we note that results of analyses and simulations may be in the range of evidentiary to indicative.

5.3 Grid Types

The data acquired by a satellite instrument constitute individual measurements per swath node (actually one measurement result per beam, overpass and swath node) and are spatially arranged in the geometry of a *swath grid*, as illustrated in Figure 2. Swath grids are dynamical (with respect to the Earth surface) because they are a projection made by the moving satellite. The Level 0 data are necessarily raster data from a swath grid. Typically, Level 1 and 2 data provided by ESA, EUMETSAT, NASA and JAXA are still in the geometry of swath grids, and annotated with time- and geo-referencing information to allow inference of time and geo-location of each swath node. Data in swath grid geometry are usually distributed as one raster per half-orbit i.e. one raster for the ascending orbit direction. The format of geo-referencing information varies; it may be given per raster as a whole or even as (latitude, longitude) coordinates per grid node.

Technically, it can be of advantage to map the swath grid nodes, onto a (spatial) *global grid*² which is uniformly and statically covering the Earth surface. Cases where mapping to a global grid is already performed at Level 1 are Nimbus-7 SSMR, DMSP SSM/I and SMOS MIRAS, and at Level 2 METOP ASCAT. Note that a global grid maps the space dimensions only, while time-referencing annotation is still maintained for the individual measurements.

Figure 4 shows the equally spaced, equal area WARP 5 global grid used for the ASCAT Level 2 SSM data. The principle of construction (indicated in the upper part of Figure 4) is as follows: a) create equally spaced latitude small circles at distances *a*, and b) on each latitude circle create grid points at discrete longitudes, again with a fixed spacing of *a*. Due to the construction the global grid has areas with irregularities. The lower part of Figure 4 shows: a) the regularity at origin, b) the divergence at the North Pole, and c) the dislocation at the 180° meridian.

² The technical term is Discrete Global Grid (DGG), however, as we do not know how a non-discrete (i.e. continuous) grid would look like, we do not use this term herein.



Figure 4: Construction of the WARP 5 Global Grid used for ASCAT L2 Data

Figure 5 a) shows the geodesic grid used for the SMOS Level 1 and Level 2 data, known as Icosahedron Snyder Equal Area (ISEA) Aperture 4 Hexagonal (ISEA4H) global grid. This grid is constructed by a subdivision method. Creating the grid involves subdividing the 20 equilateral triangles forming the faces of the regular icosahedron into more triangles, yielding 20 hexagons and 12 pentagons on the surface of the sphere (the so-called resolution 1 grid). Higher resolution grids are formed iteratively by tessellating the obtained shapes.





b) regular latitude-longitude grid used for SM ECV



Figure 5 b) shows a regular latitude-longitude grid. Grid points are equally spaced in the latitude-longitude coordinate system, however, as can be readily seen in Figure 5, they are not equally spaced / equal area on the earth surface. This grid type is utilized for the Soil Moisture ECV Data Products.

Still for technical reason, it can be of advantage to proceed further and to map the value distributions onto a *global space-time grid*. This happens usually at Level 3 because it facilitates combining data from many orbits and satellites. Satellite data mapped to a space-time grid can be viewed in two ways: For a given time index we have a raster image that can be projected to and visualized on a geographic map; for a given spatial grid point we have a timeseries that can be visualized as a graph.

		Active		Passive						
		ERS AMI- WS	METOP ASCAT	Nimb.7 SMMR	DMSP SSM/I	TRMM TMI	Aqua AMSR-E	Coriolis WindSat	SMOS MIRAS	GCOM-W1 AMSR-2
σ⁰/T _B	L1	swath	swath	EASE	EASE	swath	swath ³	swath	ISEA4H	swath
SSM	L2	WARP5	WARP5	lat-lon	lat-lon	swath	swath	swath	TBD	swath

Table 1: Grid Systems used for Calibrated Measurement Data and SSM Geophysical Parameter Data

Table 1 lists the grid types used for the Level 1 calibrated measurements of radar backscattering coefficient σ^0 and brightness temperature T_B, and the SSM geophysical parameter data.

In the process of generating the Level 3 Soil Moisture ECV Data Products, the SSM geoparameter data available in the different grid types are converted into a common space-time grid: a latitude-longitude grid (spatial resampling) and a reference time of 0:00 UTC (temporal resampling). This is the first step to produce a merged and harmonized ECV Data Product on a global and uniform space-time grid with a spatial resolution of 0.25 degree and a temporal resolution of one day.

A web-based tool to visualize and search for grid point information (e.g. geo-location, grid index, surface type) is available here: http://rs.geo.tuwien.ac.at/dv/dgg/

For more information about global grid systems cf. (Kidd 2005)] and (Bartalis 2009).

³ Product name given in [DARD] is "AMSR-E/Aqua L2A Global Swath Spatially-Resampled Brightness Temperatures", but we count it as a L1 product. The product is in swath geometry although the name seems to indicate a global grid.

5.4 Data Flow and Soil Moisture Data Processing Modules

Figure 6 shows the Soil Moisture data processing modules of Level 2 and Level 3, the latter constituting the Soil Moisture ECV Production System (ECVPS, the System). Level 1 input data are shown on the left side, the produced Level 3 ECV Data Products on the right. The arrows indicate the data flow between processing modules.



Figure 6: Principle Data Flow for the generation of Soil Moisture ECV Data Products

The overall setup of systems follows a modular design to make best use of existing European and international services, and to ensure that new satellites and instruments can be integrated. As of v04.5, SMOS has been integrated using the flexible approach; other instruments, which may be integrated in the future, include SMAP and Sentinel-1.

Level 1 calibrated measurements of (active) radar backscattering coefficient and (passive) brightness temperature, the outputs from the Level 1 processing step, are shown in Figure 6 as items in the section labelled "Level 1 Data Sets" and are available from the major providers of satellite data ESA, EUMETSAT, NASA and JAXA. A complete listing of the required Level 1 data is available in DARD [RD-7].

The conversion of the Level 1 calibrated measurements to the Level 2 Surface Soil Moisture (SSM) geo-parameter is performed individually per instrument:

- SSM parameter retrieval from the calibrated measurements of each (active) microwave scatterometer instrument is performed with the WARP change detection algorithm of TUW.
- SSM parameter retrieval from the calibrated measurements of each (passive) microwave radiometer instrument is performed with the LPRM algorithm of VUA and NASA.



SSM parameter retrieval is implemented using the established Level 2 services of EUMETSAT, NASA and JAXA that they provide for the different satellites and instruments. Descriptions of the processes can be found in DPM [RD-9] sections 4.1 and 4.2 for the active and passive cases, respectively.

The Soil Moisture ECVPS performs the final processing step, accomplished by three major modules according to Figure 6:

- Active Merging⁴: (1.) The full Level 2 SSM data set from each active instrument is resampled to a global space-time grid, (2.) each timeseries at each grid point is rescaled to the reference climatology of ASCAT, and (3.) all timeseries at each grid point are merged to a homogenised "Merged Active-only ECV Data Product".
- Passive Merging: In principle, follows the same pattern of the Active Merging, but has some extra complications (pre-processing to convert swath data into timeseries, decomposition of the AMSR-E and SSM/I timeseries into their seasonality and anomalies, incremental merging), and the rescaling is made to the reference climatology of AMSR-E, yielding a homogenised "Merged Passive-only ECV Data Product".
- Active-Passive Merging: (1.) The timeseries of the Active-only and Passive-only ECV Data Products are rescaled at each grid point to the reference climatology of "GLDAS Noah Land Surface Model L4 3 Hourly 0.25 x 0.25 degree Soil Moisture Estimate", and (2.) merged to a homogenised "Merged Active-Passive ECV Data Product".

For detailed listings and descriptions of the required Level 1 and Level 2 data cf. DARD [RD-7], for Level 2 see also SRD [RD-8] section 5 and IODD [RD-5]. The internal data flows of the Level 3 ECV generation are specified in IODD. The descriptions of the merging algorithms are in ATBD [RD-3] and (Wagner 2012). Full process descriptions of the Level 2 active and passive parameter retrieval modules and the Level 3 ECV generation modules are available in DPM [RD-9].

5.5 Soil Moisture Data Products

As an example of a Soil Moisture product, Figure 7 shows the Soil Moisture climatology for August derived from combing measurements of six satellite instruments over the period 1979 to 2010.

Surface Soil Moisture (SSM) parameter data from ERS AMI-WS and METOP ASCAT are an example of a Level 2 data product. It is retrieved from calibrated measurements of an active

⁴ Note that terms 'merging', 'blending' and 'fusion' appear in the literature, sometimes synonymously and sometimes with diversified meanings. We do not make a distinction herein and just call it 'merging'.



microwave instrument using the change detection method of TUW. The method relies upon the multi-incidence observation capabilities of the ERS and METOP scatterometers to model the effects of vegetation phenology. The SSM values are scaled between 0 and 1, representing zero Soil Moisture and saturation respectively. Parameter retrieval is not possible over tropical forest which affects about 6.5% of the land surface area.



Figure 7: Soil Moisture Anomaly for the Month August 2018

Soil Water Index (SWI) parameter data are an example of a Level 3 data product. SWI is a measure of the profile Soil Moisture content obtained by filtering the SSM timeseries with an exponential function.

Other typical examples of Level 3 products are the estimates of the Soil Moisture content for different soil layers and different temporal and spatial sampling characteristics, tailored to the needs of specific user groups.

SSM and SWI from METOP ASCAT are mapped onto a global grid and can be viewed online here: <u>http://rs.geo.tuwien.ac.at/dv/ascat/</u>



6 Specification of the products

6.1 Geophysical Parameters

The ACTIVE product is the output of merging scatterometer-based soil moisture data, which were derived from AMI-WS and ASCAT. The PASSIVE product merges data from SMMR, SSM/I, TMI, AMSR-E, WindSat, AMSR2, and SMOS. The COMBINED is directly generated from the Level 2 products used in both the ACTIVE and PASSIVE products. The data sets have been produced following the method as described by (Gruber et al. 2017; Liu et al. 2011; Wagner 2012). The SNR blending method first introduced in v03.2 of the dataset is described in (Gruber et al. 2017). The homogenised and merged products present surface soil moisture with a global coverage and a spatial resolution of 0.25°, and a temporal resolution of 1 day with a reference time at 0:00 UTC. The soil moisture data for the PASSIVE and the COMBINED product are provided in volumetric units [m³m⁻³], while the ACTIVE soil moisture data are expressed in percent of saturation [%].

6.2 Product Data Volume

The ESA CCI SM product version 04.5 is provided as global daily images, in NetCDF-4 classic file format and covers the period (yyyy-mm-dd) 1978-11-01 to 2018-12-31 for the PASSIVE and COMBINED products. The ACTIVE product covers the period from 1991-08-05 to 2018-12-31.

Product	Coverage dates	Number of files (days)	Volume size
ACTIVE	19910805 – 20181231	10012	7.05 GB
PASSIVE	19781101 – 20181231	14672	10.63 GB
COMBINED	19781101 – 20181231	14672	13.24 GB
Total	N/A	39356	30.92 GB

 Table 2 Temporal coverage and volume size of the products.

6.3 Structure and format of the product

6.3.1 Data file format and file naming

The file format used for storing the data is NetCDF-4 classic. All (NetCDF) files follow the NetCDF Climate and Forecast (CF) Metadata Conventions version 1.7. The NetCDF soil moisture data files are stored in folders for each year with one file per day. The following file naming convention, based on available CCI ECV standards, is applied:



ESACCI-<CCI Project>-<Processing Level>-<Data Type>-<Product String>[-<Additional Segregator>]-<Indicative Date>[<Indicative Time>]-fv<File version>.nc

<CCI Project>

Following the file naming convention of CCI data standards working group (DSWG) the name of this project is SOILMOISTURE.

<Processing Level>

The processing level for the ESA CCI SM products is "L3S" (super-collated), where observations from multiple instruments are combined into a space-time grid.

<Data Type>

The data type for the ACTIVE product is "**SSMS**" (surface soil moisture degree of saturation absolute), and for the PASSIVE and COMBINED product it is "**SSMV**" (surface soil moisture volumetric absolute).

<Product String>

The product string for the ACTIVE product is defined as "**ACTIVE**", for the PASSIVE product it is "**PASSIVE**", and "**COMBINED**" for the COMBINED product.

<Additional Segregator>

Additional segregator not used and not defined.

<Indicative date and time>

This field indicates the date and time for soil moisture data that are stored in the NetCDF file. The format is YYYYMMDDHHmmSS, where YYYY is the four digit year, MM is the two digit month from 01 to 12, DD is the two digit day of the month from 01 to 31, HH the two digit hour from 00 to 23, mm the two digit minute from 00 to 59, and SS the two digit second from 00 to 59. All times relate to UTC.

fv<file version>

The file version number in form xy.z provides information relating the version of the file format that has been used to provide the product. In the global NetCDF header of each data file the product version number specifies the version of the current product. Since product version 02.1 the file version and the product version number are the same.

6.3.2 NetCDF file structure

6.3.2.1 Global NetCDF Attributes

The Global NetCDF attributes are described in Table 3 for the ACTIVE, Table 4 for the PASSIVE, and Table 5 for the COMBINED product. The Global Attributes are provided for two reasons.



The attributes "**title**" and "**product version**" provide the minimum usage information about the data, whilst the remaining attributes starting with the "**summary**" attribute provide product discovery metadata for harvesting into catalogues and data federations. Because the global NetCDF attributes slightly differ between each of the three products in some points, we present the complete list of attributes.

In general, the Global Attributes will be static and not vary between files for the same file version containing the same product version, with the exception of those attributes whose content is noted by a variable; denoted as <variable>. Explicitly the following attributes will vary for every file within a product: "history" (updating creation date), "tracking id", "filename" and "date created", and between the three products, in addition to the latter, "title" (product title), "source", "time_coverage_start", "time_coverage_duration", "platform", and "sensor."

Global Attribute Name	Content
title	ESA CCI Surface Soil Moisture ACTIVE Product
institution	Technische Universität Wien (AUT), Transmissivity B.V. / VanderSat B.V. Noordwijk (NL)
contact	cci_sm_contact@eodc.eu
source	WARP 5.5R1.1/AMI-WS/ERS12 Level 2 Soil Moisture; WARP 5.4R1.0/AMI- WS/ERS2 Level 2 Soil Moisture; WARP 5.8.0/H113/ASCAT/MetOp-A DR2017 SSM time series 12.5 km sampling; WARP 5.8.0/H114/ASCAT/MetOp-A DR2018 EXT SSM time series 12.5 km sampling; WARP 5.8.0/H113/ASCAT/MetOp-B DR2017 SSM time series 12.5 km sampling; WARP 5.8.0/H114/ASCAT/MetOp-B DR2018 EXT SSM time series 12.5 km sampling
history	2019-01-21 00:00:00 - product produced
references	 http://www.esa-soilmoisture-cci.org Liu, Y.Y., Dorigo, W.A., Parinussa, R.M., de Jeu, R.A.M. , Wagner, W., McCabe, M.F., Evans, J.P., van Dijk, A.I.J.M. (2012). Trend-preserving blending of passive and active microwave soil moisture retrievals, Remote Sensing of Environment, 123, 280-297, doi: 10.1016/j.rse.2012.03.014. Liu, Y.Y., Parinussa, R.M., Dorigo, W.A., De Jeu, R.A.M., Wagner, W., van Dijk, A.I.J.M., McCabe, M.F., & Evans, J.P. (2011). Developing an improved soil moisture dataset by blending passive and active microwave satellite based retrievals. Hydrology and Earth System Sciences, 15, 425-436.

Table 3 Global NetCDF Attributes for the ACTIVE product



Global Attribute Name	Content
	Wagner, W., W. Dorigo, R. de Jeu, D. Fernandez, J. Benveniste, E. Haas, M. Ertl (2012). Fusion of active and passive microwave observations to create an Essential Climate Variable data record on soil moisture. ISPRS Annals of the Photogrammetry, Remote Sensing and Spatial Information Sciences, Volume I-7, 2012. XXII ISPRS Congress, 25 August - 01 September 2012, Melbourne, Australia.
	Gruber, A., Dorigo, W. Crow, W., & Wagner, W. (2017). Triple collocation-based merging of satellite soil moisture retrievals. IEEE Transactions on Geoscience and Remote Sensing, 1-13.
	Dorigo, W.A., Wagner, W., Albergel, C., Albrecht, F., Balsamo, G., Brocca, L., Chung, D., Ertl, M., Forkel, M., Gruber, A., Haas, E., Hamer, P. D., Hirschi, M., Ikonen, J., de Jeu, R., Kidd, R., Lahoz, W., Liu, Y. Y.,Miralles, D., Mistelbauer, T., Nicolai-Shaw, N., Parinussa, R., Pratola, C., Reimer, C., van der Schalie, R., Seneviratne, S. I. Smolander, T., Lecomte, P. (2017). ESA CCI Soil Moisture for improved Earth system understanding: State-of-the art and future directions, Remote Sensing of Environment. https://doi.org/10.1016/j.rse.2017.07.001.
tracking_id	<xxxxxxx-yyyy-zzzz-nnnn-mmmmmmmmmmmmmm (universal="" a="" identifier)="" td="" unique="" uuid="" value<=""></xxxxxxx-yyyy-zzzz-nnnn-mmmmmmmmmmmmmm>
conventions	CF-1.7
product_version	04.5
summary	The data set was produced with funding of the ESA CCI Soil Moisture and FP7- Earth2Observe projects.
keywords	Soil Moisture/Water Content
id	<filename></filename>
naming_authority	TU Wien
keywords_vocabulary	NASA Global Change Master Directory (GCMD) Science Keywords
cdm_data_type	Grid
comment	These data were produced as part of the ESA CCI Soil Moisture and FP7- Earth2Observe projects. Contract No. 4000112226/14/I-NB and GA No. 603608.
date_created	<file creation="" date=""></file>
creator_name	Department of Geodesy and Geoinformation, Technische Universität Wien (TU Wien)
creator_url	http://rs.geo.tuwien.ac.at



Global Attribute Name	Content
creator_email	cci_sm_developer@eodc.eu
project	Climate Change Initiative - European Space Agency
geospatial_lat_min	-90.0
geospatial_lat_max	90.0
geospatial_lon_min	-180.0
geospatial_lon_max	180.0
geospatial_vertical_min	0.0
geospatial_vertical_max	0.0
time_coverage_start	19910805T00000Z
time_coverage_end	20181231T00000Z
time_coverage_duration	P25Y
time_coverage_resolution	P1D
standard_name_vocabulary	NetCDF Climate and Forecast (CF) Metadata Convention
license	data use is free and open for all registered users
platform	ERS-1, ERS-2, METOP-A, Metop-B
sensor	AMI-WS, ASCAT-A, ASCAT-B
spatial_resolution	25km
geospatial_lat_units	degrees_north
geospatial_lon_units	degrees_east
geospatial_lon_resolution	0.25 degree
geospatial_lat_resolution	0.25 degree

Table 4 Global NetCDF Attributes for the PASSIVE product

Global Attribute Name	Content
Title	ESA CCI Surface Soil Moisture PASSIVE Product



Global Attribute Name	Content
institution	Technische Universität Wien (AUT), Transmissivity B.V. / VanderSat B.V. Noordwijk (NL)
contact	cci_sm_contact@eodc.eu
source	LPRMv05/SMMR/Nimbus 7 L3 Surface Soil Moisture, Ancillary Params, and quality flags; LPRMv05/SSMI/F08, F11, F13 DMSP L3 Surface Soil Moisture, Ancillary Params, and quality flags; LPRMv05/TMI/TRMM L2 Surface Soil Moisture, Ancillary Params, and QC; LPRMv06/AMSR-E/Aqua L2B Surface Soil Moisture, Ancillary Params, and QC; LPRMv05/WINDSAT/CORIOLIS L2 Surface Soil Moisture, Ancillary Params, and QC; LPRMv06/AMSR2/GCOM-W1 L3 Surface Soil Moisture, Ancillary Params; LPRMv06/SMOS/MIRAS L3 Surface Soil Moisture, CATDS Level 3 Brightness Temperatures (L3TB) version 300 RE03 & RE04
history	2019-01-21 12:00:00 - product produced
references	 http://www.esa-soilmoisture-cci.org Liu, Y.Y., Dorigo, W.A., Parinussa, R.M., de Jeu, R.A.M., Wagner, W., McCabe, M.F., Evans, J.P., van Dijk, A.I.J.M. (2012). Trend-preserving blending of passive and active microwave soil moisture retrievals, Remote Sensing of Environment, 123, 280-297, doi: 10.1016/j.rse.2012.03.014. Liu, Y.Y., Parinussa, R.M., Dorigo, W.A., De Jeu, R.A.M., Wagner, W., van Dijk,
	A.I.J.M., McCabe, M.F., & Evans, J.P. (2011). Developing an improved soil moisture dataset by blending passive and active microwave satellite based retrievals. Hydrology and Earth System Sciences, 15, 425-436.
	Wagner, W., W. Dorigo, R. de Jeu, D. Fernandez, J. Benveniste, E. Haas, M. Ertl (2012). Fusion of active and passive microwave observations to create an Essential Climate Variable data record on soil moisture. ISPRS Annals of the Photogrammetry, Remote Sensing and Spatial Information Sciences, Volume I-7, 2012. XXII ISPRS Congress, 25 August - 01 September 2012, Melbourne, Australia.
	Gruber, A., Dorigo, W. Crow, W., & Wagner, W. (2017). Triple collocation-based merging of satellite soil moisture retrievals. IEEE Transactions on Geoscience and Remote Sensing, 1-13.
	Dorigo, W.A., Wagner, W., Albergel, C., Albrecht, F., Balsamo, G., Brocca, L., Chung, D., Ertl, M., Forkel, M., Gruber, A., Haas, E., Hamer, P. D., Hirschi, M., Ikonen, J., de Jeu, R., Kidd, R., Lahoz, W., Liu, Y. Y., Miralles, D., Mistelbauer, T., Nicolai-Shaw, N., Parinussa, R., Pratola, C., Reimer, C., van der Schalie, R., Seneviratne, S. I. Smolander, T., Lecomte, P. (2017). ESA CCI Soil Moisture for



Global Attribute Name	Content
	improved Earth system understanding: State-of-the art and future directions, Remote Sensing of Environment. https://doi.org/10.1016/j.rse.2017.07.001.
tracking_id	<xxxxxxx-yyyy-zzzz-nnnn-mmmmmmmmmmmmmm (universal="" a="" unique<br="" uuid="">Identifier) value</xxxxxxx-yyyy-zzzz-nnnn-mmmmmmmmmmmmmm>
conventions	CF-1.7
product_version	04.5
summary	These data were produced as part of the ESA CCI Soil Moisture and FP7- Earth2Observe projects. Contract No. 4000112226/14/I-NB and GA No. 603608.
keywords	Soil Moisture/Water Content
id	<filename></filename>
naming_authority	TU Wien
keywords_vocabulary	NASA Global Change Master Directory (GCMD) Science Keywords
cdm_data_type	Grid
comment	These data were produced as part of the ESA CCI Soil Moisture and FP7- Earth2Observe projects. Contract No. 4000112226/14/I-NB and GA No. 603608.
date_created	<file creation="" date=""></file>
creator_name	Department of Geodesy and Geoinformation, Technische Universität Wien (TU Wien)
creator_url	http://rs.geo.tuwien.ac.at
creator_email	cci_sm_developer@eodc.eu
project	Climate Change Initiative - European Space Agency
geospatial_lat_min	-90.0
geospatial_lat_max	90.0
geospatial_lon_min	-180.0
geospatial_lon_max	180.0
geospatial_vertical_min	0.0
geospatial_vertical_max	0.0
time_coverage_start	19781101T000000Z



Global Attribute Name	Content
time_coverage_end	20181231T000000Z
time_coverage_duration	P38Y
time_coverage_resolution	P1D
standard_name_vocabulary	NetCDF Climate and Forecast (CF) Metadata Convention
license	data use is free and open for all registered users
platform	Nimbus 7, DMSP, TRMM, AQUA, Coriolis, GCOM-W1, MIRAS
sensor	SMMR, SSM/I, TMI, AMSR-E, WindSat, AMSR2, SMOS
spatial_resolution	25km
geospatial_lat_units	degrees_north
geospatial_lon_units	degrees_east
geospatial_lon_resolution	0.25 degree
geospatial_lat_resolution	0.25 degree

Table 5 Global NetCDF Attributes for the COMBINED product

Global Attribute Name	Content
Title	ESA CCI Surface Soil Moisture COMBINED Product
institution	Technische Universität Wien (AUT), Transmissivity B.V. / VanderSat B.V. Noordwijk (NL)
contact	cci_sm_contact@eodc.eu
source	WARP 5.5R1.1/AMI-WS/ERS12 Level 2 Soil Moisture; WARP 5.8.0/H113/ASCAT/MetOp-A DR2017 SSM time series 12.5 km sampling; WARP 5.8.0/H114/ASCAT/MetOp-A DR2018 EXT SSM time series 12.5 km sampling; WARP 5.8.0/H113/ASCAT/MetOp-B DR2017 SSM time series 12.5 km sampling; WARP 5.8.0/H114/ASCAT/MetOp-B DR2018 EXT SSM time series 12.5 km sampling; LPRMv05/SMMR/Nimbus 7 L3 Surface Soil Moisture, Ancillary Params, and quality flags; LPRMv05/SSMI/F08, F11, F13 DMSP L3 Surface Soil Moisture, Ancillary Params, and quality flags; LPRMv05/TMI/TRMM L2 Surface Soil Moisture,
	Ancillary Params, and QC; LPRMv06/AMSR-E/Aqua L2B Surface Soil Moisture, Ancillary Params, and QC; LPRMv05/WINDSAT/CORIOLIS L2 Surface Soil Moisture, Ancillary Params, and QC; LPRMv06/AMSR2/GCOM-W1 L3 Surface Soil



Global Attribute Name	Content
	Moisture, Ancillary Params; LPRMv06/SMOS/MIRAS L3 Surface Soil Moisture, CATDS Level 3 Brightness Temperatures (L3TB) version 300 RE03 & RE04
history	2019-01-21 00:00:00 - product produced
references	http://www.esa-soilmoisture-cci.org
	Liu, Y.Y., Dorigo, W.A., Parinussa, R.M., de Jeu, R.A.M., Wagner, W., McCabe, M.F., Evans, J.P., van Dijk, A.I.J.M. (2012). Trend-preserving blending of passive and active microwave soil moisture retrievals, Remote Sensing of Environment, 123, 280-297, doi: 10.1016/j.rse.2012.03.014.
	Liu, Y.Y., Parinussa, R.M., Dorigo, W.A., De Jeu, R.A.M., Wagner, W., van Dijk, A.I.J.M., McCabe, M.F., & Evans, J.P. (2011). Developing an improved soil moisture dataset by blending passive and active microwave satellite based retrievals. Hydrology and Earth System Sciences, 15, 425-436.
	Wagner, W., W. Dorigo, R. de Jeu, D. Fernandez, J. Benveniste, E. Haas, M. Ertl (2012). Fusion of active and passive microwave observations to create an Essential Climate Variable data record on soil moisture. ISPRS Annals of the Photogrammetry, Remote Sensing and Spatial Information Sciences, Volume I-7, 2012. XXII ISPRS Congress, 25 August - 01 September 2012, Melbourne, Australia.
	Gruber, A., Dorigo, W. Crow, W., & Wagner, W. (2017). Triple collocation-based merging of satellite soil moisture retrievals. IEEE Transactions on Geoscience and Remote Sensing, 1-13.
	Dorigo, W.A., Wagner, W., Albergel, C., Albrecht, F., Balsamo, G., Brocca, L., Chung, D., Ertl, M., Forkel, M., Gruber, A., Haas, E., Hamer, P. D., Hirschi, M., Ikonen, J., de Jeu, R., Kidd, R., Lahoz, W., Liu, Y. Y.,Miralles, D., Mistelbauer, T., Nicolai-Shaw, N., Parinussa, R., Pratola, C., Reimer, C., van der Schalie, R., Seneviratne, S. I. Smolander, T., Lecomte, P. (2017). ESA CCI Soil Moisture for improved Earth system understanding: State-of-the art and future directions, Remote Sensing of Environment. https://doi.org/10.1016/j.rse.2017.07.001.
tracking_id	<xxxxxxx-yyyy-zzzz-nnnn-mmmmmmmmmmmmmm (universal="" a="" unique<br="" uuid="">Identifier) value</xxxxxxx-yyyy-zzzz-nnnn-mmmmmmmmmmmmmm>
conventions	CF-1.7
product_version	04.5
summary	These data were produced as part of the ESA CCI Soil Moisture and FP7- Earth2Observe projects. Contract No. 4000112226/14/I-NB and GA No. 603608.



Global Attribute Name	Content
keywords	Soil Moisture/Water Content
id	<filename></filename>
naming_authority	TU Wien
keywords_vocabulary	NASA Global Change Master Directory (GCMD) Science Keywords
cdm_data_type	Grid
comment	These data were produced as part of the ESA CCI Soil Moisture and FP7- Earth2Observe projects. Contract No. 4000112226/14/I-NB and GA No. 603608.
date_created	<file creation="" date=""></file>
creator_name	Department of Geodesy and Geoinformation Technische Universität Wien (TU Wien)
creator_url	http://rs.geo.tuwien.ac.at
creator_email	cci_sm_developer@eodc.eu
project	Climate Change Initiative - European Space Agency
geospatial_lat_min	-90.0
geospatial_lat_max	90.0
geospatial_lon_min	-180.0
geospatial_lon_max	180.0
geospatial_vertical_min	0.0
geospatial_vertical_max	0.0
time_coverage_start	19781101T00000Z
time_coverage_end	20181231T000000Z
time_coverage_duration	P38Y
time_coverage_resolution	P1D
standard_name_vocabulary	NetCDF Climate and Forecast (CF) Metadata Convention
license	data use is free and open for all registered users
platform	Nimbus 7, DMSP, TRMM, ERS-1, ERS-2, METOP-A, AQUA, Coriolis, GCOM-W1, MIRAS
sensor	SMMR, SSM/I, TMI, AMI-WS, ASCAT, AMSR-E, WindSat, AMSR2, SMOS


Global Attribute Name	Content
spatial_resolution	25km
geospatial_lat_units	degrees_north
geospatial_lon_units	degrees_east
geospatial_lon_resolution	0.25 degree
geospatial_lat_resolution	0.25 degree



6.3.2.2 NetCDF Data File Variables and Attributes

lon

Table 6 Attribute Table for Variable lon

NetCDF Attribute	Description
standard_name	longitude
units	degrees_east
valid_range	[-180.0, 180.0]
_CoordinateAxisType	Lon

lat

Table 7 Attribute Table for Variable Lat

NetCDF Attribute	Description
standard_name	latitude
units	degrees_north
valid_range	[-90.0, 90.0]
_CoordinateAxisType	Lat

time

Table 8 Attribute Table for Variable time (reference time). The type of this variable is double.

NetCDF Attribute	Description
standard_name	Time
units	days since 1970-01-01 00:00:00 UTC
calendar	Standard
_CoordinateAxisType	Time



sm (ACTIVE product)

Table 9 Attribute Table for Variable sm for the ACTIVE product

NetCDF Attribute	Description
long_name	Percent of Saturation Soil Moisture
units	percent
_CoordinateAxes	lat lon time
_FillValue	-9999.0 (NaN); type: float32 (4 bytes)

sm (PASSIVE and COMBINED product)

Table 10 Attribute Table for Variable sm for the PASSIVE and COMBINED products

NetCDF Attribute	Description
long_name	Volumetric Soil Moisture
units	m ³ m ⁻³
_CoordinateAxes	lat lon time
_FillValue	-9999.0 (NaN); type: float32 (4 bytes)

sm_uncertainty (ACTIVE product)

Table 11 Attribute Table for Variable sm_noise

NetCDF Attribute	Description
long_name	Percent of Saturation Soil Moisture Uncertainty
Units	percent
_CoordinateAxes	lat lon time
_FillValue	-9999.0 (NaN); type: float32 (4 bytes)

sm_uncertainty (PASSIVE and COMBINED product)

Table 12 Attribute Table for Variable sm_uncertainty for the PASSIVE and COMBINED products

NetCDF Attribute	Description
long_name	Volumetric Soil Moisture Uncertainty
Units	m3 m-3
_CoordinateAxes	lat lon time
_FillValue	-9999.0 (NaN); type: float32 (4 bytes)

dnflag

Table 13 Attribute Table for Variable dnflag

NetCDF Attribute	Description
long_name	Day / Night Flag
flag_values	[0, 1, 2, 3]
flag_meanings	0 = NaN 1 = day 2 = night 3 = combination of day and night
_CoordinateAxes	lat lon time
_FillValue	0 (NaN); type: signed byte



flag

Table 14 Attribute Table for Variable flag

NetCDF Attribute	Description			
long_name	Flag			
flag_values	[0, 1, 2, 3, 4, 5, 6, 7, 127]			
flag_meanings	0 = no_data_inconsistency_detected			
	1 = snow_coverage_or_temperature_below_zero			
	2 = dense_vegetation			
	3 = combination of flag values 1 and 2			
	4 = others_no_convergence_in_the_model_thus_no_valid_sm_estimates			
	5 = combination of flag values 1 and 4			
	6 = combination of flag value 2 and 4			
	7 = combination of flag values 1, 2, and 4			
_CoordinateAxes	lat lon time			
_FillValue	127 (NaN); type: signed byte			



freqbandID

Table 15 Attribute Table for Variable freqbandID

NetCDF Attribute	Description				
long_name	Frequency Band Identification				
flag_values	[0, 1, 2, 3, 4, 8, 9, 10, 11, 16, 17, 18, 19, 24, 25, 26, 27, 32, 33, 34, 35, 64, 65, 66, 67, 72, 73, 74, 75, 80, 81, 82, 83, 128, 130]				
flag_meanings	Binary Decimal 0000000 0 0000000 0 0000000 0 0000000 0 0000000 0 0000000 0 0000000 0 0000000 0 0000000 0 0000000 0 0000000 0 0000000 0 0000000 0 0000000 0 0000000 1 0000000 2 00000000 32 01000000 128 Sensors and their operating SMMR SSM/I TMI AMSR-E AMSR2 6.9 WindSat SMOS AMI-WS ASCAT-A/B	Value Mea 19 L14+C53+C 24 C68+C69 25 L14+C68+C 26 C53+C68+C 32 C73 33 L14+C73 34 C53+C73 35 L14+C73 34 C53+C73 35 L14+C73 34 C53+C73 35 L14+C3+C 64 X107 65 L14+X107 66 C53+K107 d the correspondiu Frequency [GHz] NaN 1.4 5.3 / 5.255 6.6 6.8 6.9 / 6.93 7.3 10.65 / 10.7 19.35 / 19.4 19.35 10.65 / 10.7 19.35 10.65 / 10.7 19.35 10.65 / 10.7 19.35 10.65 / 10.7 19.35 10.65 / 10.7 19.35 6.8 / 10.7 1.4 5.3 / 7.3 / 10.65 5 6.8 / 10.7 1.4	ning 69 69 69 68+C69 73 73 73 73 73 73 73 73 73 73	Value 67 72 73 74 75 80 81 82 83 128 130 M A A A A A A A A A A A A A	Meaning L14+C53+X107 C68+X107 L14+C68+X107 C53+C68+X107 L14+C53+C68+X107 C69+X107 L14+C69+X107 C53+C69+X107 L14+C53+C69+X107 K194 C53+K194
_CoordinateAxes	lat lon time				
_FillValue	0 (NaN); type: signed i	nteger			



mode

Table 16 Attribute Table for Variable mode

NetCDF Attribute	Description
long_name	Satellite Mode
flag_values	[0, 1, 2, 3]
flag_meanings	0 = NaN 1 = ascending 2 = descending 3 = combination of ascending and descending
_CoordinateAxes	lat lon time
_FillValue	0 (NaN); type: signed byte

sensor

Table 17 Attribute Table for Variable sensor

NetCDF Attribute	Description		
long_name	Sensor		
flag_values	[0, 1, 2, 4, 8, 16, 24, 32, 64, 72, 80, 88, 96, 128, 130, 132, 136, 256, 264, 272, 280, 288, 320, 328, 336, 344, 352, 512, 544, 576, 608, 768, 800, 832, 864]		
flag_meanings	ValueSensor Combination0NaN264AMSRE+ASCATA1SMMR272WindSat+ASCATA2SSMI280AMSRE+WindSat+ASCATA4TMI288AMSRE+WindSat+ASCATA8AMSRE320SMOS+ASCATA16WindSat328AMSRE+SMOS+ASCATA24AMSRE+WindSat336WindSat+SMOS+ASCATA32AMSR2344AMSRE+WindSat+SMOS+ASCATA64SMOS352AMSR2+SMOS+ASCATA72AMSRE+SMOS512ASCATB80WindSat+SMOS576SMOS+ASCATB96AMSR2+SMOS608AMSR2+ASCATB130SSMI+AMIWS768ASCATA+ASCATB132TMI+AMIWS800AMSR2+ASCATA132SMIE+AMIWS864AMSR2+ASCATB256ASCATA864AMSR2+SMOS+ASCATA+ASCATB		
_CoordinateAxes	lat lon time		
_FillValue	0 (NaN); type: signed integer		



t0

Table 18 Attribute Table for Variable t0

NetCDF Attribute	Description
long_name	Observation Time Stamp
units	days since 1970-01-01 00:00:00 UTC
valid_range	<individual decimal="" depending="" numbers="" observation="" on="" timestamp=""></individual>
_CoordinateAxes	lat lon time
_FillValue	-9999.0; type: double

6.4 Annotation datasets

The surface soil moisture data (sm) are generated by blending passive and active microwave soil moisture retrievals. The data provided are in percentage of saturation [%] units for the ACTIVE product, and volumetric [m³m⁻³] units for the PASSIVE and COMBINED products. Quality Flags and Indicators.

6.4.1 sm_uncertainty

The merging of soil moisture data from different sensors requires a harmonization of the data. The data need to be brought into a common climatology by running them through several scaling procedures performing the cumulative distribution function (CDF-) matching technique. The provided "sm_uncertainty" parameter represents the error variance of the data sets (in the respective climatology of the dataset), estimated through triple collocation (TC) analysis. In periods where TC cannot be applied, or in cases where the TC-based error variance estimates do not converge, sm_uncertainty is set to NaN. The unit of sm_uncertainty for the ACTIVE product is percentage of saturation [%]. For the PASSIVE and the COMBINED product the unit is volumetric [m³m⁻³]. For the ACTIVE and the PASSIVE products, the error variance is directly estimated using TC analysis. For the COMBINED product, these estimates are propagated through the SNR blending model using a standard error propagation scheme.

Product	Time Period
ACTIVE	1991-08-05 to 2018-12-31
PASSIVE	1987-07-09 to 2018-12-31
COMBINED	1987-07-09 to 2018-12-31

 Table 19 sm_uncertainty data provided in the ESA CCI SM Products



6.4.2 dnflag

The Day or Night Flag gives information, whether the observation(s) occurred at local day (1) or night (2) time. A value of 3 indicates that the data is a result of merging satellite microwave data observed during day as well as during night time. In cases where the information cannot be determined the value is set to 0 (zero).

6.4.3 flag

Flag values are stored as signed bytes, and the default value (NaN, not a number) is 127. By reading the flag for the surface soil moisture data, the user gets information for that grid point. A "0" (zero) informs that the sm value for that grid point has been checked, but there was no inconsistency found. A "1" denotes, that the soil for that location is covered with snow or the temperature is below zero. Reading a "2" indicates that the observed location is covered by dense vegetation, and a "4" stands for all other cases, e.g. no convergence in the model, thus no valid soil moisture estimates.

6.4.4 freqbandID

The surface soil moisture data has its sources from multiple and different satellite sensors, which operate in various frequencies. The freqbandID values are representing the operating frequencies and comprise the combination of different frequency bands. Table 15 lists these combinations.

6.4.5 mode

The NetCDF variable mode stores the information of the sensor's orbit direction. Ascending direction are denoted as 1, and descending orbit as 2. In cases where the orbit direction cannot be determined, the NaN value 0 (zero) is used. A value of 3 means that the merged data comprises both ascending and descending satellite modes.

6.4.6 sensor

The values for sensor are stored as signed integer, with NaN as 0 (zero). These values indicate the satellite sensors that have been used for a specific grid point. Valid values range from 1 to 864. Table 17 list all available sensor combinations.



6.4.7 t0

The original observation timestamp is stored within the NetCDF variable t0 (t-naught). Time values coming from two different sensors are averaged. Values of -9999.0 are used as NaN values. t0 data values are stored as number of "days since 1970-01-01 00:00:00 UTC" (see Table 18).

6.4.8 time

The reference timestamp of the day is saved in the "time" variable. The data values for the reference time are stored as number of "days since 1970-01-01 00:00:00 UTC"

6.5 Product Grid and Projection

The grid is a 0.25° x 0.25° longitude-latitude global array of points, based on the World Geodetic System 1984 (WGS 84) reference system. Its dimension is 1440 x 720, where the first dimension, X (longitude) is incrementing most rapidly West (-180°) to East (180°), and the second dimension, Y (latitude) is incrementing South (-90°) to North (90°). Grid edges are at multiple of quarter-degree values (e.g. 90, 89.75, 89.5, 89.25, ...), and the grid centers are exactly between two grid edges:

First point centre = (-89.875°S, -179.875°W) = Grid Point Index = 0 Second point centre = (-89.875°S, -179.625°W) = Grid Point Index = 1 1441st point centre = (-89.625°S, -179.875°W) = Grid Point Index = 1440 Last point centre = (89.875°N, 179.875°E) = Grid Point Index = 1036799

In total, there are $1440 \times 720 = 1036800$ grid points, where 244243 points are land points. Figure 8 shows the land points that are used for the merged product.



Figure 8: Land mask used for the merged product. The 0.25° grid starts indexing from "lower left" to the "upper right". Note that not every grid points are available for all sensors, e.g. ASCAT retrievals are available between Latitude degrees 80° and –60°.

7 ESA CCI SM in Earth system applications

The following section is taken from (Gruber et al. 2017) as is presents the broadest review to date of the current use and application of the ESA CCI SM product by the wider scientific community. The exhaustive list of references for this section are presented in Section 12.

The use of ESA CCI SM products in a wide variety of studies helps improve our understanding of Earth system processes (Table 20), in particular with respect to climate variability and change. Even though the application fields are seemingly different, in all of them ESA CCI SM plays a central role in benchmarking, calibrating, or providing an alternative to the land surface hydrology in dedicated models. The following sections will provide an extensive synthesis of how ESA CCI SM has been used so far in the different application areas and what potential still remains unexploited.

Table 20: Applications where ESA CCI SM has been used to improve our Earth system understanding.Modified from Dorigo and De Jeu (2016).

Application area	Main purpose	References
Climate variability and	Long-term trends in soil moisture	(Albergel et al. 2013; An et al. 2016; Dorigo et al. 2012; Qiu et al. 2016b; Rahmani et al. 2016; Su et al. 2016; Wang et al. 2016)
change	Assessment of drivers of soil moisture trends	(Feng 2016; Liu et al. 2015)



	Soil moisture as driver of multi-annual variability in land evaporation	(Miralles et al. 2014b)
	Impact of ocean atmosphere system on soil moisture variability	(Bauer-Marschallinger et al. 2013; Miralles et al. 2014b; Nicolai-Shaw et al. 2016)
	Soil moisture as indicator of global climate variability and change	(De Jeu et al. 2011; De Jeu et al. 2012; Dorigo et al. 2014; Dorigo et al. 2015a; Dorigo et al. 2016; Parinussa et al. 2013)
	Impact of soil moisture trends on atmospheric composition	(Klingmüller et al. 2016)
	Validation of climate model runs	(Du et al. 2016; Lauer et al. 2017; Pieczka et al. 2016)
	Improved understanding of soil moisture feedbacks on precipitation	(Guillod et al. 2014; Guillod et al. 2015) (indirectly, through assimilation of ESA CCI SM into GLEAM)
Land atmosphere	Identifying role of soil moisture on temperature variability and heatwaves	(Casagrande et al. 2015; Hirschi et al. 2014; Miralles et al. 2014a)
interactions	Improved modelling of land evaporation	(Martens et al. 2017; Miralles et al. 2014b)
	Impact of soil moisture on dust and aerosols	(Klingmüller et al. 2016)
	Benchmarking and calibrating global vegetation models	(Szczypta et al. 2014; Traore et al. 2014)
Global biogeochemical	Impact of soil moisture dynamics on vegetation productivity	Barichivich et al. (2014); Chen et al. (2014); McNally et al. (2016); Muñoz et al. (2014); Nicolai-Shaw et al. (2016); Papagiannopoulou et al. (2017a); Papagiannopoulou et al. (2017b); Szczypta et al. (2014)
	Connecting trends in soil moisture and vegetation productivity	(Dorigo et al. 2012; Feng 2016)
	Improved crop modelling	(Sakai et al. ; Wang et al. 2016)
	Assessing drivers of fire activity	(Charles et al. 2016; Forkel et al. 2016)
Hydrology and land surface	Benchmarking model <i>states</i> in hydrological and land surface models	(Du et al. 2016; Fang et al. 2016; Lauer et al. 2017; Loew et al. 2013; Schellekens et al. 2017; Spennemann et al. 2015; Szczypta et al. 2014)
modelling	Benchmarking model <i>processes</i> in hydrological and land surface models (e.g. dry down)	(Chen et al. 2016)



	Persistence and prediction of soil moisture anomalies in land surface models	(Nicolai-Shaw et al. 2016)
	Improving runoff predictions and flood (risk) modelling	(Massari et al. 2015; Tramblay et al. 2014)
	Improved water budget modelling	(Abera et al. 2016; Allam et al. 2016)
	Assessing irrigation	(Kumar et al. 2015; Qiu et al. 2016b)
	Assessing the impact of agricultural intensification on soil moisture	(Liu et al. 2015)
	Computing cumulative precipitation amounts	(Ciabatta et al. 2016)
	Validation of drought indices	(van der Schrier et al. 2013)
Drought	Development of new drought index	(Carrão et al. 2016; Enenkel et al. 2016; Rahmani et al. 2016)
applications	Improved detection of agricultural droughts	(Liu et al. 2015; Yuan et al. 2015)
	Soil moisture for integrated drought monitoring	(Enenkel et al. 2016; McNally et al. 2016; Nicolai-Shaw et al. 2016; Rahmani et al. 2016)
Meteorological applications	Improving NWP land surface scheme	This study (Section 7.6)

7.1 Assessing climate variability and change

As soil moisture is an integrative component of the Earth system, any large scale variability or change in our climate should manifest itself in globally observed patterns. In this role, ESA CCI SM has made a significant contribution to the body of evidence of natural and human-induced climate variability and change. Emblematic for this is the contribution of ESA CCI SM to the State of the Climate Reports that are issued every year by National Oceanic and Atmospheric Administration (e.g., Blunden and Arndt 2016).

Several studies have shown a clear relationship between major oceanic-atmospheric modes of variability in the climate system, e.g. El Niño Southern Oscillation (ENSO), and variations in ESA CCI SM (Bauer-Marschallinger et al. 2013; Dorigo et al. 2016; Miralles et al. 2014b; Nicolai-Shaw et al. 2016). By applying enhanced statistical methods to the multi-decadal ESA CCI SM v0.1 dataset over Australia, Bauer-Marschallinger et al. (2013) were able to disentangle the portion of soil moisture variability that is driven by the major climate oscillations affecting this continent, i.e., ENSO, the Indian Ocean Dipole and the Antarctic Oscillation, from other modes



of short-term and long-term variability. Miralles et al. (2014b) showed that inter-annual soil moisture variability as observed by ESA CCI SM COMBINED v02.2 largely drives the observed large-scale variability in continental evaporation.

ESA CCI SM has been widely used to assess global trends in soil moisture, mostly in combination with LSMs. Based on ESA CCI SM v0.1 (Dorigo et al. 2012) computed that for the period 1988–2010 27% of the area covered by the dataset showed significant trends, of which almost three quarters were drying trends. The strong tendency towards drying were largely confirmed by trends computed for the same period from ERA-Interim and GLDAS-Noah (Dorigo et al. 2012), and ERA-Interim/Land and MERRA-Land (Albergel et al. 2013), although the spatial trend patterns were not everywhere congruent between datasets. The agreement in trends between a newer version of ESA CCI SM (v02.2) and MERRA-Land were recently confirmed by Su et al. (2016). Trend analyses performed on a more regional scale, but for different time periods (An et al. 2016; Rahmani et al. 2016; Wang et al. 2016) generally confirmed the results obtained at the global scale while providing a more detailed view on the impact of local land management practices, e.g. irrigation, on observed trends (Qiu et al. 2016b), and the impact of soil moisture trends in regional climate (Klingmüller et al. 2016). Feng (2016) made an assessment of the drivers of trends in ESA CCI SM COMBINED v02.2 soil moisture and concluded that at the global scale climate change is by far the most important driver of changes in soil moisture, although at the regional level vegetation change may play a significant role. Nevertheless, given the limitations in record lengths, the impact of lowfrequency climate oscillations on trends should first be carefully addressed before any robust conclusion about the sign and magnitude of the trend can be drawn (Miralles et al. 2014b). Likewise, the potential impact of dataset artefacts should be carefully quantified and corrected for (Su et al. 2016).

7.2 Land-atmosphere interactions

As soil moisture is essential in partitioning the fluxes of water and energy at the land surface, it can affect the dynamics of humidity and temperature in the lower troposphere. This control of soil moisture on evapotranspiration is important for the intensity and persistence of heatwaves, as the depletion of soil moisture and the resulting reduction in evaporative cooling may trigger an amplified increase in air temperature (Fischer et al. 2007b; Hirschi et al. 2011; Miralles et al. 2014a; Seneviratne et al. 2006c). While many studies on soil moisture– evapotranspiration and soil moisture–temperature coupling are based on modelling results or use precipitation-based drought indices as a proxy for soil moisture, ESA CCI SM enables analyses based on long-term soil moisture estimates (Hirschi et al. 2014; Miralles et al. 2014a). The 2003 heatwave in Europe and the 2010 heatwave in Russia both showed distinct negative anomalies in ESA CCI SM v02.1 during the heatwaves, amplifying the lack of evaporative cooling and favouring the progressive build-up of atmospheric heat in the atmospheric



boundary layer (Miralles et al. 2014a). Moreover, the temporal evolution and timing of periods of extreme dry soil moisture conditions in ESA CCI SM COMBINED v02.2 coincide well with anomalies in evapotranspiration, temperature, and fAPAR (Nicolai-Shaw et al. 2016).

Limitations with respect to the depth of the soil moisture retrievals (i.e., reporting the content of moisture in the first few centimetres as opposed to the entire root depth affecting transpiration) have triggered some debate about its appropriateness to investigate evapotranspiration dynamics and atmospheric feedbacks (Hirschi et al. 2014). Hirschi et al. (2014) showed that the strength of the relationship between soil moisture and temperature extremes appears underestimated with ESA CCI SM remote sensing-based surface soil moisture compared to estimates based on the Standardized Precipitation Index (SPI; McKee et al. 1993; Stagge et al. 2015). This is related to an underestimation of the temporal dynamics and of large dry/wet anomalies within ESA CCI SM. This effect is enhanced under extreme dry conditions and may lead to a decoupling of the surface layer from deeper layers and from atmospheric fluxes (and resulting temperatures). Thus the added value of root-zone soil moisture is likely more important for applications dealing with extreme conditions, while for mean climatological applications the information content in the surface layer appears adequate. In addition, the importance of having root-zone soil moisture information also seems to depend on the application. For example, (Qiu et al. 2016a) showed that the prediction of near-future vegetation anomalies profits from vertically integrated soil moisture (as an approximation of root-zone soil moisture) as opposed to surface soil moisture alone. In a later study however they found no clear evidence that using vertically extrapolated soil moisture as opposed to surface soil moisture observations enhances the estimation of surface energy fluxes (Qiu et al. 2016a). The assimilation of remote sensing surface soil moisture into a land surface model (e.g., Lannoy and Reichle 2016) provides a possible alternative here. In fact, root zone soil moisture estimates by the satellite-based Global Land Evaporation Amsterdam Model (GLEAM; Miralles et al. 2011) are already improved by the assimilation of ESA CCI SM, while the overall quality of evaporation estimates remains similar after assimilation (Martens et al. 2017). Also, the assimilation of ESA CCI SM COMBINED v02.1 helped interpreting global land evaporation patterns and multi-annual variability in response to the El Niño Southern Oscillation (Miralles et al. 2014b).

Soil moisture also affects precipitation through evapotranspiration. Yet, the effect of soil moisture on precipitation is much more debated than for air temperature. Studies report both positive or negative feedbacks, and even no feedback. Using a precursor of ESA CCI SM, Taylor et al. (2012) identified a spatially negative feedback of soil moisture on convective precipitation regarding the location, i.e., that afternoon rain is more likely over relatively dry soils due to mesoscale circulation effects. Guillod et al. (2015) revisited the soil moisture effect on precipitation using GLEAM root-zone soil moisture with ESA CCI SM COMBINED v02.1 assimilated, and showed that spatial and temporal correlations with opposite signs may



coexist within the same region: precipitation events take place preferentially during wet periods (moisture recycling), but within the area have a preference to fall over comparatively drier patches (local, spatially negative feedbacks).

A more indirect but potentially strong soil moisture – atmosphere feedback was found by Klingmüller et al. (2016), who were able to link an observed positive trend in Aerosol Optical Depth (AOD) in the Middle East to a negative trend in ESA CCI SM COMBINED v02.1. As lower soil moisture translates into enhanced dust emissions, their results suggested that increasing temperature and decreasing relative humidity in the last decade have promoted soil drying, leading to increased dust emissions and AOD. These changes in atmospheric composition again may have considerable impact on radiative forcing and precipitation initiation (Ramanathan et al. 2001) and as such impact the energy and water cycles in the area.

7.3 Global biogeochemical cycles

Soil moisture is a regulator for various processes in terrestrial ecosystems such as plant phenology, photosynthesis, biomass allocation, turnover, and mortality; and the accumulation and decomposition of carbon in soils (Carvalhais et al. 2014; Nemani et al. 2003; Reichstein et al. 2013; Richardson et al. 2013). Low soil moisture during drought reduces photosynthesis, enhances ecosystem disturbances such as insect infestations or fires, and thus causes plant mortality and accumulation of dead biomass in litter and soils (Allen et al. 2010; McDowell et al. 2011; Thurner et al. 2016). The release of carbon from soils to the atmosphere through respiration is also controlled by soil moisture (Reichstein and Beer, 2008). Consequently, soil moisture is a strong control on variations in the global carbon cycle (Ahlström et al. 2013; Poulter et al. 2014; van der Molen et al. 2012).

Despite the importance of soil moisture for the global carbon cycle, satellite-derived soil moisture data is currently under-explored in carbon cycle and ecosystem research. Because long-term soil moisture observations were lacking until recently, most studies on the effects of soil moisture on vegetation relied on precipitation estimates (Du et al. 2013; Poulter et al. 2013), indirect drought indices (Hogg et al. 2013; Ji and Peters 2003), or soil moisture estimates from land surface models (Forkel et al. 2015; Rahmani et al. 2016). More recently, authors used ESA CCI SM to assess impacts of water availability and droughts on plant phenology and productivity based on satellite-derived vegetation indices such as the Normalized Difference Vegetation Index (NDVI) or the Leaf Area Index (LAI). For example, Szczypta et al. (2014) used ESA CCI SM v0.1, modelled soil moisture, and LAI over the Euro-Mediterranean zone to evaluate two land surface models and to predict LAI anomalies over cropland. LAI was predictable from ESA CCI SM in large homogeneous cropland regions, e.g. in Southern Russia (Szczypta et al. 2014). Strong positive relationships between ESA CCI SM COMBINED and NDVI were also found for Australia (Chen et al. 2014; v0.1), for croplands in the North China plains (Wang et al. 2016; v0.1), and for East Africa (McNally et al. 2016; v0.2.1).



Generally, many regions with positive (greening) or negative (browning) trends in NDVI show also positive and negative trends in ESA CCI SM v0.1, respectively (Dorigo et al. 2012). This cooccurrence of soil moisture and NDVI trends reflects the strong water control on vegetation phenology and productivity. Interestingly, soil moisture from ESA CCI SM v0.1 was also correlated with NDVI in some boreal forests which are primarily temperature-controlled (Barichivich et al. 2014). In these regions, soil moisture and vegetation productivity were controlled by variations in the accumulation and thawing of winter snow packs (Barichivich et al. 2014). However, some water-limited regions had negative EAA CCI SM v0.1 soil moisture trends with no corresponding trend in NDVI (Dorigo et al. 2012). In these cases, the positive relation between surface soil moisture and vegetation is likely modified by vegetation type and vegetation density (Feng, 2016; McNally et al., 2016). For example, densely vegetated areas in East Africa show stronger correlations between ESA CCI SM COMBINED v02.1 soil moisture and NDVI than sparsely vegetated areas (McNally et al., 2016). Novel data-driven approaches allow to assess the share of ESA CCI SM in controlling NDVI variability as opposed to other water and climate drivers (Papagiannopoulou et al. (2017a); Papagiannopoulou et al. (2017b)). Figure 9 shows the correlation between the latest ESA CCI SM COMBINED (v03.2) product and NDVI GIMMS 3G (Tucker et al. 2005) with a lag time of soil moisture preceding NDVI of 16 days. In most regions and especially in water-limited areas such as the Sahel, there is a strong and direct response of NDVI to soil moisture. On the other hand, correlations are negative in many temperate regions. This is likely due to the fact that NDVI is highest in summer months when soil moisture decreases. This demonstrates that vegetation productivity in temperate regions is primarily temperature-controlled and strongly affected by human activities through agriculture or forest management (Forkel et al. (2015); Papagiannopoulou et al. (2017b)).

Apart from the analysis of relations with vegetation indices, the ESA CCI SM datasets have been occasionally used in other ecosystem studies. For example, Muñoz et al. (2014) investigated tree ring chronologies of Conifers in the Andeans in conjunction with soil moisture variability from ESA CCI SM v0.1. The study revealed a previously unobserved relation between tree growth and summer soil moisture (Muñoz et al., 2014). Furthermore, ESA CCI SM v0.1 and vegetation data were used to evaluate ecosystem models (Szczypta et al. 2014; Traore et al. 2014). Thereby, the results of Traore et al. (2014) demonstrate that a model that best performs for soil moisture does not necessarily best perform for plant productivity. This demonstrates the need to jointly use soil moisture and vegetation or carbon cycle observations to improve global ecosystem/carbon cycle models (Kaminski et al. 2013). For example, SMOS soil moisture data and observations of atmospheric CO₂ have been used to estimate parameters of a global vegetation model within a carbon cycle data assimilation system (Scholze et al. 2016). The use of the ESA CCI SM in such an analysis could potentially constrain model uncertainties regarding the long-term hydrological control on vegetation productivity and ecosystem respiration. However, a major source of uncertainty about the



future terrestrial carbon cycle is related to how global ecosystem models represent carbon turnover, vegetation dynamics, and disturbances such as fires (Friend et al. 2014). It was previously shown that variations in satellite-derived soil moisture are related to extreme fire events in boreal forests (Bartsch et al. 2009; Forkel et al. 2012). Consequently, the ESA CCI SM COMBINED dataset has been used together with climate, vegetation, and socio-economic data to assess controls on fire activity globally and to identify appropriate structures for global fire models (Charles et al. 2016; Forkel et al. 2016).



Figure 9: Mean Pearson correlation coefficient R between ESA CCI soil moisture v03.1 and GIMMS NDVI3g for the period 1991 to 2013 for a lag time of soil moisture preceding NDVI by 16 days.

7.4 Hydrological and land surface modelling

As soil moisture drives processes like runoff, flooding, evaporation, infiltration, and ground water recharge, it is important for hydrological models to accurately map soil moisture states. The potential of using ESA CCI SM to validate surface soil moisture fields in state-of-the-art LSMs, reanalysis products, and large-scale hydrological models has been largely recognized (Fang et al. 2016; Loew et al. 2013; Spennemann et al. 2015; Szczypta et al. 2014). Schellekens et al. (2017) exploited the long-term availability of ESA CCI SM COMBINED v02.2 to validate according to a standardised protocol the soil moisture fields of ten global hydrological and land surface models, all forced with the same meteorological forcing dataset for the period 1979-2012. In a similar systematic way, ESA CCI SM COMBINED (v0.1 and v02.2, respectively) was used to evaluate the model outputs of CMIP (Du et al. 2016; Lauer et al. 2017). New insights in the model representation of hydrological processes like infiltration have been offered by comparing the memory length (Chen et al. 2016) and the frequency domains (Polcher et al. 2016) between LSMs and remote sensing products, including ESA CCI SM COMBINED v02.3.

Satellite soil moisture data can bring important benefits in run-off modelling and forecasting both through an improved initialisation of rainfall-runoff models and through data



assimilation techniques that allow for updating the soil moisture states. Several studies have shown the positive impact on flood and runoff prediction through assimilation of single sensor soil moisture products, e.g. obtained from ASCAT (Brocca et al. 2010), AMSR-E (Sahoo et al. 2013), and SMOS (Lievens et al. 2015). Wanders et al. (2014) and Alvarez-Garreton et al. (2015) showed the improved skill when jointly assimilating multiple soil moisture products (SMOS, ASCAT and AMSR-E), resulting mainly from improved temporal sampling. Long-term homogeneous soil moisture products like ESA CCI SM become important in flood modelling studies that require a multi-year period for the calibration and validation of model parameters. Assimilating the ESA CCI SM COMBINED v02.2 product over the Upper Niger River basin improved run-off predictions even though the simulation of the rainfall-runoff model was already good (Massari et al. 2015). Tramblay et al. (2014) used the ESA CCI SM product to better constrain model parameters, and hence reduce uncertainties, of a parsimonious hydrological model in the Mono River basin (Africa), with the goal to evaluate the impact of climate change on extreme events. Further studies are clearly needed to assess the full potential of ESA CCI SM product for run-off modelling and forecasting. For example, even a simple model based only on persistence allows for the prediction of soil moisture (Nicolai-Shaw et al. 2016), and exploiting this characteristic could contibute to improved early warning systems.

ESA CCI SM and its Level 2 input products have been used for improving the quantification of the different components of the hydrological cycle, i.e. evaporation (Allam et al. 2016; Martens et al. 2017; Miralles et al. 2014b), groundwater storage (Abelen and Seitz 2013), and rainfall (Ciabatta et al. 2016). Due to its ability to serve as a temporary water reservoir, soil moisture contains information on antecedent precipitation. This principle is being exploited by the SM2RAIN method (Brocca et al. 2014; Brocca et al. 2013), which uses an inversion of the soil-water balance equation to obtain a simple analytical relationship for estimating precipitation accumulations from the knowledge of a soil moisture time-series. The method has been tested on a wide range of Level 2 satellite soil moisture products and ESA CCI SM COMBINED v02.2 (Brocca et al. 2014; Ciabatta et al. 2016). SM2RAIN realistically reproduces daily precipitation amounts when compared to gauge observations and in certain regions may even perform better than state-of-the-art direct satellite observations of precipitation, even though its performance hinges on the quality of the soil moisture product used as input (Brocca et al. 2014; Ciabatta et al. 2016). Its application to ESA CCI SM COMBINED provides an independent global climatology of precipitation from 1979 onwards. Abera et al. (2016) used the SM2RAIN precipitation product from ESA CCI SM (Ciabatta et al. 2016) to quantify the space-time variability of rainfall, evaporation, runoff and water storage for the Upper Blue Nile river basin in Africa.

ESA CCI SM has also been used to map irrigation, which, is largely unquantified on a global scale and, consequently, not included in most large scale hydrological and/or land surface



models (Qiu et al. 2016b). Kumar et al. (2015) used satellite soil moisture observations from ESA CCI SM COMBINED v02.1, ASCAT, AMSR-E, SMOS, and Windsat for the detection of irrigation over United States. By comparing modelled and satellite soil moisture data, irrigated areas can be detected when satellite data and modelled data (the latter do not include irrigation) show different temporal dynamics. Similarly, Qiu et al. (2016b) detected irrigated areas in China by evaluating the differences in trends between ESA CCI SM COMBINED v02.1 and precipitation, and Liu et al. (2015) use ESA CCI SM v0.1 to support the attribution of the aggravating droughts in Northern China to an increase in fertilizer application.

7.5 Drought applications

Soil moisture or agricultural droughts are related to periods of water deficits, and can be driven by a lack of precipitation and/or increased evapotranspiration (Seneviratne et al. 2012). In addition to natural causes, human influences such as poor water management and bad land practices can initiate or exacerbate drought conditions (Liu et al. 2015; Van Loon et al. 2016). Until recently, global soil moisture observations were scarce, which favoured the use of available meteorological observations, such as precipitation and temperature, to develop indices for drought monitoring. Well-known examples, although primarily indicative of meteorological drought rather than soil moisture or agricultural drought, are the SPI and the Palmer Drought Severity Index (PDSI; Palmer 1965).

ESA CCI SM can be used to directly monitor soil moisture or agricultural drought, or help to set up alternative drought indicators. For example, Carrão et al. (2016) and Rahmani et al. (2016) used ESA CCI SM COMBINED (v02.0 and v02.1, respectively) to develop a drought index comparable to SPI but based on actual soil moisture observations instead of precipitation, naming them the Empirical Standardized Soil Moisture Index (ESSMI) and Standardized Soil Moisture Index (SSI), respectively. Carrão et al. (2016) found high correlations between ESSMI and maize, soybean and wheat crop yields in South-Central America and with this index could accurately describe the severe and extreme drought intensities in north-eastern Brazil in 1993, 2012, and 2013. Based on SSI, Rahmani et al. (2016) were able to identify a severe drought event that started in December 2012 in the northern part of the Iran. The Enhanced Combined Drought Index (ECDI) as proposed by Enenkel et al. (2016) combines ESA CCI SM COMBINED v02.2 with satellite-derived observations of rainfall, land surface temperature and vegetation vigour for the detection of drought events, and has been successfully used to detect large-scale drought events in Ethiopia between the years 1992-2014.

McNally et al. (2016) specifically evaluated the use of ESA CCI SM COMBINED v02.2 for agricultural drought and food security monitoring in East Africa, and found that remotely sensed soil moisture is a valuable addition to a 'convergence of evidence' framework for drought monitoring. Like Dorigo et al. (2015b) they emphasize that users should be aware of the spatial and temporal differences in data quality caused for example by significant data

gaps prior to 1992, the lack of overlap between sensors, or difficulties with soil moisture retrievals over certain terrains such as heavily vegetated areas. Post 1992 McNally et al. (2016) generally found good agreement between ESA CCI SM and other soil moisture products as well as with NDVI in East Africa. (Yuan et al. 2015) assessed the skill of ESA CCI SM v02.1 in capturing short-term soil moisture droughts over China. They found that the PASSIVE and COMBINED products have better drought detection skills over the sparsely vegetated regions in north-western China while ACTIVE worked best in eastern China. At the global scale Miralles et al. (2014b) identified the effect of El Niño-driven droughts in soil moisture, NDVI and evaporation, using GLEAM and ESA CCI SM COMBINED v02.1. Relationships between extreme dry soil conditions, derived from the ESA CCI SM COMBINED v02.2 dataset, and temperature, precipitation, evapotranspiration and vegetation activity were also found by Nicolai-Shaw et al. (2016). This in combination with the high persistence of soil moisture (Nicolai-Shaw et al. 2016; Seneviratne et al. 2006a) makes the ESA CCI SM dataset valuable for the prediction and monitoring of drought events.

7.6 Meteorological applications

soil moisture

Numerical Weather Prediction (NWP) involves the use of computer models of the Earth system to simulate how the state of the Earth system is likely to evolve over a period of few hours up to 1-2 weeks ahead. It also considers longer timescales (seasonal and climate) through the notion of seamless prediction (Palmer et al. 2008). A number of studies provide strong support for the notion that high skill in short- and medium-range forecasts of air temperature and humidity over land requires proper initialization of soil moisture (Beljaars et al. 1996; Douville et al. 2000; Drusch and Viterbo 2007; van den Hurk et al. 2012). There is evidence also of a similar impact from soil moisture on seasonal forecasts (Koster et al. 2011; Koster et al. 2004b; Weisheimer et al. 2011).

Remotely sensed soil moisture datasets like ESA CCI SM can serve NWP in two ways. First, they can offer a long-term, consistent, and independent reference against which NWP output fields can be evaluated. This may eventually improve meteorological forecasts through a better representation of the land surface, and improved representation of the fluxes between the land surface and the atmosphere in the NWP (see Section 7.2). Recently, ECMWF made an offline development in its Land Surface Model HTESSEL (Balsamo et al. 2015; Balsamo et al. 2009), making it possible to add extra layers of soil as well as changing their thickness. An experiment was run which increases the number of soil layers from four to nine and reduces the thickness of the upper soil layer from seven (0-7 cm) to one (0-1) centimetre. One of the rationales for having this thin topsoil layer is having a surface layer that is closer to the depth sampled by existing satellite observations and thus allowing for a better assimilation of these observations. Soil moisture from the first layer of two offline experiments, forced by ERA-Interim reanalysis, and considering either a 1 cm depth (GE8F) or a 7 cm depth (GA89) layer



was compared to the ESA CCI SM COMBINED v02.2 over 1979-2014. Correlations were computed for absolute soil moisture and anomaly time series from a 35-day moving average (Dorigo et al. 2015b). We illustrate differences in correlation between the two experiments in Figure 10. The predominant red colours illustrate that in most areas using a surface layer 1 instead of 7 cm depth leads to a better match with the ESA CCI SM COMBINED dataset. Positive differences frequently reach values higher than 0.2, particularly for correlations on anomaly time series, which shows that a thinner model layer better mimics surface soil moisture variations, as was expected.



-0.30 -0.24 -0.18 -0.12 -0.06 0 0.06 0.12 0.18 0.24 0.30

Figure 10 : Differences in correlations of absolute soil moisture values (left) and anomalies (right) differences between ESA CCI SM and soil moisture from the first layer of soil of two offline experiments over 1979-2014. Experiment GE8F has a first layer of soil of 1 cm depth (0-1cm), GA89 of 7 cm depth (0-7cm).

Only few studies have assimilated remotely-sensed soil moisture directly into NWPs and climate models to update their soil moisture fields. Even though this mostly leads to a significant improvement of the model's soil moisture fields, its impact on the meteorological forecast itself, e.g. on 2 metre air temperature (Bisselink et al. 2011), screen temperature or relative humidity predictions (de Rosnay et al. 2013; Dharssi et al. 2011; Scipal et al. 2008), is typically limited in areas with dense coverage of the ground-based meteorological observing network and difficult to evaluate in poorly observed areas.

8 Known Issues and Limitations

The known issues and limitations for the ECV SM 04.5 product are briefly provided in the following section. All issues and limitations are fully addressed in the corresponding ATBD for the product in sections "known limitations" and "scientific advances under investigation".

8.1 Passive ECV product

The known limitations in deriving soil moisture from passive microwave observations are listed and described in detail in this section. These issue do not only apply to the current CCI



soil moisture dataset release but also to soil moisture retrieval from passive microwave observations in general.

8.1.1 Vegetation

Vegetation affects the microwave emission, and under a sufficiently dense canopy the emitted soil radiation will become completely masked by the overlaying vegetation. The simultaneously derived vegetation optical depth can be used to detect areas with excessive vegetation, of which the boundary varies with observation frequency. Figure 11 gives an example of the relationship between the analytical error estimate in soil moisture as described in the previous section and vegetation optical depth. This figure shows larger error values in the retrieved soil moisture product for higher frequencies at similar vegetation optical depth values. For example, for a specific agricultural crop (VOD=0.5), the error estimate for the soil moisture retrieval in the C-band is around 0.07 m³·m⁻³; in the X-band, this is around 0.11 m³·m⁻³, and in the Ku-band, this is around 0.16 m³·m⁻³. All relevant frequency bands show an increasing error with increasing vegetation optical depth. This is consistent with theoretical predictions, which indicate that, as the vegetation biomass increases, the observed soil emission decreases, and therefore, the soil moisture information contained in the microwave signal decreases Owe et al. (2001). In addition, retrievals from the higher frequency observations (i.e., X- and Ku-bands) show adverse influence by a much thinner vegetation cover. Soil Moisture retrievals with a soil moisture error estimates beyond 0.2 m³m⁻³ are considered to be unreliable and are masked out



Figure 11: Error of soil moisture as related to the vegetation optical depth for 3 different frequency bands (from Parinussa et al. (2011)).

For the new L-band based retrievals from SMOS, the vegetation influence is less as compared to the C-, X- and Ku-band retrievals, which can be seen from the R_{value} and Triple Collocation Analysis (TCA) results in Figure 12. In Figure 12, the SMOS LPRM and AMSR-E LPRM (based on C-band) are included and shows more stable results over dense vegetation, i.e. NDVI values of over 0.45. A complete analysis on the error for L-band soil moisture, comparable to the results from Figure 11, are planned in the future.



Figure 12: Triple Collocation Analysis (TCA: top) and Rvalue results (bottom) for several soil moisture datasets, including SMOS LPRM and AMSR-E LPRM, for changing vegetation density (NDVI). Based on van der Schalie et al. (2018).

8.1.2 Frozen surfaces and snow

Under frozen surface conditions the dielectric properties of the water changes dramatically and therefore all pixels where the surface temperature is observed to be at or below 273 K



are assigned with an appropriate data flag, this was determined using the method of Holmes et al. (2009).

8.1.3 Water bodies

Water bodies within the satellite footprint can strongly affect the observed brightness temperature due to the high dielectric properties of water. Especially when the size of a water body changes over time they can dominate the signal. LPRM uses a 5 % water body threshold based on MODIS observations and pixels with more than 5 % surface water are masked.

8.1.4 Rainfall

Rainstorms during the satellite overpass affect the brightness temperature observation, and are therefore flagged in LPRM. The flagging system for active rain is based on the rainfall index of Seto et al. (2005). This method makes use of the vertical polarized 36.5 GHz and 19 GHz observations to detect a rain event. Index values of 5 and beyond are used to identify an active rainstorm. Soil moisture retrievals with these index values are flagged.

8.1.5 Radio Frequency interference

Natural emission in several low frequency bands are affected by artificial sources, so called Radio Frequency Interference (RFI). As a diagnostic for possible errors an RFI index is calculated according to Nijs et al. (2015). Most passive microwave sensors that are used for soil moisture retrieval observe in several frequencies. This allows LPRM to switch to higher frequencies in areas affected by RFI. The new methodology that is now used for RFI detection uses the estimation of the standard error between two different frequencies. It uses both the correlation coefficient between two observations and the individual standard deviation to determine the standard error in Kelvin. A threshold value of 3 Kelvin is used to detect RFI. This method does not produce false positives in extreme environments and is more sensitive to weak RFI signals in relation to the traditional methods (e.g. Li et al. (2004)).

As the currently integrated SMOS mission does not have multiple frequencies to apply this method, here we base the filtering on the RFI probability information that is supplied by in the SMOS Level 3 data.

8.2 Active ECV Product

8.2.1 Computation of Slope/Curvature Parameters

Another line of investigation we shall start is the feasibility of estimating slope/curvature values separately for each year (instead of inter-annually). This was clearly not possible for

ERS, but even for ASCAT with its increased temporal resolution the question remains if under these conditions enough data remains within the time window to yield reliable parameter estimates. An interesting aspect would be the possibility to detect slope-outliers (e.g., due to extraordinary events like flash-floods or drought) by comparing the slope estimates for the same day across several years. These outliers would be removed before computing an interannually averaged slope parameter which will be used in all cases where a full processing is either deemed too costly (periodic time series append without reprocessing of parameters at TU Wien) or simply not possible (WARP NRT running at EUMETSAT).

8.2.2 Dry and Wet Crossover Angles

The crossover angle concept states that at the dry and wet crossover angles, vegetation has no effect on backscatter (Wagner et al. (1999)). These crossover angles have been determined empirically based on four study areas (Iberian Peninsula, Ukraine, Mali, and Canadian Prairies). Nevertheless, the empirically determined dry and wet crossover angles are used on a global scale in the surface soil moisture retrieval model. A known limitation of the global use of these crossover angles is that depending on the vegetation type - or more precisely the evolution of biomass of a specific vegetation type -, crossover angles may vary across the globe, which is not yet considered in the model. Furthermore, for some regions on the Earth's surface the crossover angle concept may not be applicable, in particular regions without vegetation cover (i.e., deserts).

8.2.3 Backscatter in Arid Regions

In arid regions or more specifically in desert environments it appears that the dry reference shows seasonal variations, which are assumed to reflect vegetation phenology. But this cannot be true for desert environments which are characterised by very limited or no vegetation at all. In principle, seasonal variations of the dry reference are desirable to account for backscatter changes induced by vegetation referred to as vegetation correction. Vegetation correction is based upon changes in the slope parameter, which can be also observed in desert environment. These variations seem to have a big impact particularly in areas with very low backscatter. Hence, it needs to be clarified whether it is a real physical process, noise or something else reflected in the slope parameter.

8.3 Combined Active + Passive ECV Product

The current product version combining the active and passive ECVs into a merged active/passive ECV is based on data availability (at a daily time step) and their sensitivity to vegetation. For most locations, either only the rescaled passive merged data set or the rescaled active merged data set is used, based on a threshold in vegetation optical depth



obtained from LPRM retrievals. Despite the growing number of satellites available for soil moisture retrieval, data gaps or lower observation densities arise over large parts of Eurasia, South America, and Africa. The static merging framework adopted for CCI SM production, which either uses passive products (over sparsely vegetated areas), active products (moderately vegetated areas) or both (intermediately vegetated areas), does currently not allow for filling such gaps with lower quality observations. It is currently being investigated how the static merging scheme can be alleviated to fill such gaps without making compromise with respect to the overall product quality. Using a weighted merging scheme based on triple collocation based signal-to-noise estimates is the most likely candidate to follow up the static merging scheme (Gruber et al. 2017).

In order to verify if the quality of the merged product is comparable to or better than that of the individual input products, (Gruber et al. 2017) validated the version 0.1 over 596 in-situ stations of the ISMN and compared these results with the evaluation results obtained for the individual contributing products. It was observed that for the active products there is not as much of an improvement in correlation as that observed for most of the passive data sets. The cause of this is still not entirely clear, but is most likely related to the higher spatial resolution of the ASCAT product and the non-optimal scaling resulting from this discrepancy in scale.

8.4 Passive merged CCI product

8.4.1 Using night-time observations only

For the current version of the merged passive product only descending overpasses, corresponding to night-time / early morning observations, were considered. This is because near surface land surface temperature gradients are regarded to be reduced at night leading to more robust retrievals (Owe et al. 2008). However, recent studies (Brocca et al. 2011) suggest that for specific land cover types day-time observations may provide more robust retrievals than night-time observations, although the exact causes are still unknown. If day-time observations could be introduced to the blended product, this would significantly increase the observation density.

8.5 Intercalibration of AMSR-E and AMSR2

As AMSR-E stopped delivering data on 04 October 2011, the continuity of the passive radiometer data is prolonged by using the WindSat and AMSR2 data sets. The Passive product is extended by using WindSat to bridge the time gap between AMSR-E and AMSR2. A intercalibration technique was developed to adjust WindSat soil moisture to AMSR-E and AMSR2 to the adjusted Windsat data (Parinussa et al. 2015). However, the overlapping period use to compute the calibration constants was very short and need to be updated using a larger



time window. Alternatively, JAXA announced to make an improved intercalibrated AMSR2 product available, which, if outperforming the empirical intercalibration used so far, will be used to generate level 2 AMSR2 LPRM soil moisture estimates.

8.6 Active Product

8.6.1 Intercalibration of ERS and ASCAT

The generation of the ERS and ASCAT products is still based on their individual time series. The merged ERS + ASCAT could significantly profit from an appropriate Level 1 intercalibration. Besides improving the quality of the individual measurements this would improve the robustness of the calculation of the dry and wet references.

8.6.2 Data gaps

Similar as for the passive products, merging ERS and ASCAT into a merged dataset is based on a strict separation in time. Gaps in ASCAT time series can be potentially filled with ERS observations, although the spatial and temporal overlap between both sensors is limited.

9 Data Access and Acknowledgements

9.1 Data Access

The active, passive and merged products are freely available for download after the completion of a simple user registration and the users approval by the CCI SM team data administrators. User registration is available at:

http://www.esa-soilmoisture-cci.org/dataregistration

Registration is required to deter automated systems having direct access to the product. Data downloaded by the registered user can be used by the user and the associated organisation, no onward distribution is permitted.

The current product version is ECV SM v04.5. If you are interested in previous product versions, please send us a request. Our contact details are provided in Section 9.3.

The data set is also available via ESA's open data portal: <u>http://cci.esa.int/data</u>

9.2 Data Reader

The esa_cci_sm Python package available on the TU Wien GEO GitHub repository (<u>https://github.com/TUW-GEO/esa_cci_sm</u>) provides readers for the ESA CCI soil moisture



datasets (images and time series within the "interface" module). It also allows conversion of daily images to gridded time series via the "reshuffle" module. The README.rst file contains information about installation of the package. Please contact the CCI SM team for advice on using the reader.

9.3 Contact

The CCI SM team can be contact directly via <u>cci sm contact@eodc.eu</u>.

E-mails sent to this address reaches both data managers and key project scientists.

9.4 Scientific use only

The ECV SM product is intended for scientific purposes only.

9.5 No onward distribution

Re-export or transfer of the original data (as received from the ECV SM sftp) by the data users to a third party is prohibited. This is in the best interest of both the individual data providers and the potential users as unrestricted copying of the original data by multiple, independent users may lead to errors in the data.

9.6 Intellectual Property Rights

User acknowledges the respective data owner's full title and ownership of the data and nothing in these terms and conditions shall be construed as granting or implying any rights to, or interest in copyrights or intellectual property rights of the respective data owners.

9.7 Acknowledgement and citation

Whenever the product, made available by the CCI SM project, is used for publication, the data's origin (i.e. the CCI SM project) must be acknowledged and referenced.

The data set should be cited using the complete references as follows:

- Gruber, A. Scanlon, T., van der Schalie, R., Wagner, W., Dorigo, W. (2019) Evolution of the ESA CCI Soil Moisture Climate Data Records and their underlying merging methodology. Earth System Science Data 11, 717-739, https://doi.org/10.5194/essd-11-717-2019
- Gruber, A., Dorigo, W. Crow, W., & Wagner, W. (2017). Triple collocation-based merging of satellite soil moisture retrievals. IEEE Transactions on Geoscience and Remote Sensing, 1-13. https://doi.org/10.1109/TGRS.2017.2734070.



Dorigo, W.A., Wagner, W., Albergel, C., Albrecht, F., Balsamo, G., Brocca, L., Chung, D., ٠ Ertl, M., Forkel, M., Gruber, A., Haas, E., Hamer, P. D., Hirschi, M., Ikonen, J., de Jeu, R., Kidd, R., Lahoz, W., Liu, Y. Y., Miralles, D., Mistelbauer, T., Nicolai-Shaw, N., Parinussa, R., Pratola, C., Reimer, C., van der Schalie, R., Seneviratne, S. I. Smolander, T., Lecomte, P. (2017). ESA CCI Soil Moisture for improved Earth system understanding: State-ofart Environment. and future directions, Remote Sensing the of https://doi.org/10.1016/j.rse.2017.07.001.

9.8 User feedback

Use feedback is warmly welcomed and encouraged. All questions and remarks concerning the product can be addressed to our contact e-mail address provided in Section 9.3.

10 Terminology of Remote Sensing and Earth Observation

Table 21 lists the prime business domain terms from the scientific and technological domains of remote sensing, satellite-based Earth Observation and Soil Moisture retrieval.

Term (Acronym)	Description	Synonyms
Remote sensing	Is the acquisition of information about an object or phenomenon without making physical contact with the object. There are two main types of remote sensing: passive remote sensing and active remote sensing, corresponding to active and passive instruments, respectively (see below).	
Sensed object	The object subject of a remote sensing activity.	Sensed target Sensed system
Instrument	In the given context: An imaging microwave instrument flying onboard of an earth observation satellite. The instrument is a payload of the satellite. In a wide sense: Any device that can be used to perform a measurement.	Sensor Measureme nt device
Active instrument	An instrument that uses its own source of electromagnetic energy for the measurement.	
Scatterometer	An active microwave instrument, measuring the radar backscattering coefficient σ^0 in physical units [dB] or [m ² /m ²].	Radar
Passive instrument	An instrument that measures energy that is reflected or emitted from the sensed object.	
Radiometer	A passive microwave instrument, measuring the brightness temperature T_{B} in physical unit [K].	

Table 21: Business Domain Terminology: Remote Sensing, Earth Observation, Soil Moisture



Term (Acronym)	Description	Synonyms
Beam	The direction sensed by single antennae; used to express the fact that a satellite instrument may have several antennas each with its own field of view (FOV).	
Satellite	In the given context always means Earth Observation (EO) satellite.	
Orbit	The path of a satellite on its way around the earth.	
Single overpass Single orbit	The term is used to stress the fact that a satellite instrument scans only once across the earth surface and makes a single or a tuple of measurements per swath node.	Single scan
	Implies that individual beams contributing to a measurement result are synchronized to the sensed object.	
Revisiting orbit	The term is used to stress the fact that measurements of a satellite instrument were not made in a single overpass.	Overlapping orbits Multi-pass orbits
Swath	The area of the earth surface along the ground track of a satellite that is sensed by the instrument in a single overpass; has a definite width but indefinite begin an end; made of an explicit number of nodes in the width-dimension that repeat in regular intervals along the direction of the ground track; each node is the sensed object of a single or a tuple of measurements.	
L <n></n>	Processing levels L0 to L4 are an organization of the chain of	
Level Processing Level	data processing performed on the payload data from EO satellites.	
Merging	Process of combining the measurements or retrievals from revisiting orbits of a satellite or from many satellites with the aim to reach an improved coverage of the observed domain in space or time. Terms 'merging', 'blending' and 'fusion' appear in the literature sometimes synonymously and sometimes with diversified meanings.	Blending Fusion
Grid	Narrow: A set of nodes, lines or areas in a two-dimensional space that are arranged in a repeated pattern; may result from a construction principle or an actual process that repeats in regular intervals. Wide: Extended to n-dimensional space, and to space-time.	
Node	One point (or area) out of a set of similar points (areas) that together form a grid.	
Grid type	Classification of grids by construction principle.	



Term (Acronym)	Description	Synonyms
Swath grid	The grid originating from a satellite instrument when it senses the individual areas of the earth surface in a repetitive pattern during a single overpass; each grid node represents a single or a tuple of measurements. A swath grid is the result of the projection made by the instrument's beams; images in swath grid are in the perspective of the instrument's point of view (POV). Nodes of revisiting orbits do not coincide, thus swath grids are dynamic and not statically linked to the earth surface.	Data in orbit geometry. Data in instrument projection. Image in the perspective of the instrument's point of view
Global grid	A spatial grid that is uniformly and statically covering the earth surface.	(POV). Discrete Global Grid
	Some global grids use a geoid model (e.g. WGS84 reference ellipsoid) to account for the earth's oblateness. Swath grids can be mapped onto global rids by means of a spatial resampling.	(DGG) (Global) grid system
Global space- time grid	The Cartesian product of a global grid and a timeseries index.	
Geo-referencing	Linkage of grid nodes to points of the earth surface; expressed in latitude and longitude coordinates. Geo-referencing parameters (e.g. satellite ephemeris) allow linking measurement results with the remotely sensed objects on the land surface.	
Time referencing	Linkage of a timeseries index (e.g. swath nodes) to UTC time.	
Measurement	The process of experimentally obtaining one or more quantity values that can reasonably be attributed to a quantity.	Observation
Quantity	A property of a phenomenon, body, or substance, where the property can take on a value that can be expressed as a number and a reference.	Observable Variable
Quantity value	A pair of number and reference, together expressing the value of a quantity.	
Reference	A reference can be a measurement unit, a measurement procedure, a reference material, or a combination of such.	Scale
Measurand	A quantity that is intended to be measured.	
Calibration	An operation performed for an instrument that establishes a relation between measurement standards and the quantity values and uncertainties indicated by the instrument. In case of L1 data, radiometric and geometric calibration coefficients may be either attached (L1a) or applied (L1b).	
Distribution	A function that assigns values to the points of a space, time or space-time domain; the assignment may be continuous or discrete, e.g. to the points of a grid.	
Domain	The range in space, time or space-time that is designated for value assignment.	



Term (Acronym)	Description	Synonyms
Coverage	The fraction of the domain where values have been actually assigned.	
Raster	A two-dimensional array; every element is accessible by the pair of row and column index, is called a pixel, and contains a single or a tuple of values.	Image Raster image
Pixel	An element of a raster.	
Timeseries	A one-dimensional vector; every element is accessible by an index and contains a single or a tuple of values; the index represents points or periods in time that are sampled in equal (or near-equal) intervals.	
Physical system	A part of nature chosen for analysis. The part outside the system is its environment. Effects of the environment on the system are taken into account by an abstraction, and vice- versa. The cut between system and environment is a free choice, generally made to simplify analysis. An isolated system is one which has negligible interaction with its environment.	Geo-physical system
Parameter	A measurable quantity suited to express the state of a physical system. In the given context synonymous for "geophysical parameter".	Sate variable Geophysical parameter Environment al Variable
Local parameter	Characterizes the state of a local and compact object in space (i.e. a local physical system). A Local parameter may be measureable with remote sensing instruments, while others may not be measurable with such instruments, but can still be inferred from direct measurements and additional knowledge about the sensed system (retrieval by an inversion or modelling approach).	Local state variable
Model	A relation between parameters of a physical system, expressed in a mathematical or computable manner. E.g. as an equation system, $Y = f(X)$, where X and Y being tuples of system parameters; or as a computer simulation.	Mathematic al model Simulation
Retrieval	The process of obtaining parameter values of a physical system from remote sensing measurements, although the parameters cannot be directly measured (observed) with the used remote sensing instruments. A retrieval is made on a mathematical-physical basis as follows: (1) It is known that at any time quantities X and quantities Y have definite values; (2) it is known that there exists a functional relation between system parameters X and instrument observables Y; (3) there is partial knowledge about the functional relation, e.g. in the form of a forward model Y = f(X) or an inversion X = $g(Y)$; and (4) under certain conditions the knowledge of the functional relation is sufficient to determine X from the measurements of Y.	Parameter retrieval



Term (Acronym)	Description	Synonyms
Retrieval algorithm	The algorithm (or approach, or method) used to retrieve a parameter value from remote sensing measurements.	Retrieval approach or method
Surface Soil Moisture (SSM)	A local geophysical parameter expressing the content of water in the top soil surface layer (of < 2 cm thickness), in physical units [%] or $[m^3/m^3]$. Typical SSM data products from global satellite observations have a spatial resolution of 25x25 km. Regional products downscaled with use of SAR data are available in a resolution of 1x1 km.	
TUW change detection algorithm	The algorithm used to retrieve the SSM parameter from calibrated measurements of the radar backscattering coefficient σ^0 made by an (active) scatterometer microwave instrument. Uses climate data timeseries of seasonally varying dry and wet reference values. Developed at TUW; implemented by the WARP processing module.	
Land Parameter Retrieval Model (LPRM)	An iterative forward modelling approach used to retrieve the SSM parameter from calibrated measurements of the brightness temperature T_B made by a (passive) radiometer microwave instrument. Uses a global database of physical soil properties. Developed by NASA and VUA.	
Soil Water Index (SWI)	A measure of the profile Soil Moisture content of soil surface layers within 2-100 cm obtained by using an infiltration model (filtering the SSM timeseries with an exponential function).	
Climate	Climate is a measure of the average pattern of variation of meteorological variables (e.g. temperature, humidity, atmospheric pressure, wind, precipitation, atmospheric particle count, etc.) in a given region over long periods of time. A region's climate is generated by the climate system, which has five components: atmosphere, hydrosphere, cryosphere, land surface, and biosphere.	
Essential Climate Variable (ECV)	Essential Climate Variables are geophysical parameters that are required to support the work of the United Nations Framework Convention on Climate Change (UNFCCC), and that are technically and economically feasible for systematic observation. An ECV Data Product combines observations from multiple remote-sensing instruments into a space-time grid; is complete and consistent, with a global and continuing coverage; and is intended for use in climate modeling. Synonyms are Super-collated (L3S) Data and TCDR.	L3S Thematic Climate Data Record (TCDR)
Climatology	Average of a geophysical parameter for a given region; obtained from long-term (many year) observation.	
Seasonality	Seasonal variation of a parameter's climatology, e.g. variation over the months of a year.	



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