EUMETSAT Satellite Application Facility on
Support to Operational Hydrology and Water Management
http://hsaf.meteoam.it/

Algorithm Theoretical Baseline Document (ATBD) H141 and H142

Soil Wetness Index in the roots region
Data Record and Offline extension

Revision History

Revision	Date	Author(s)	Description
0.1	2019/05/07	David Fairbairn and Patricia de Rosnay	First draft.
0.2	2019/11/06	David Fairbairn and Patricia de Rosnay	(i) Revised Table 4.1 to provide the correct producers and references of the H141 input scatterometer SSM products; (ii) The product name is now included in the title of the document; (iii) Information about the quality control screening of the input scatterometer observations has been added in section 4.1.1
0.3	2020/03/12	David Fairbairn and Patricia de Rosnay	(i) Included descriptions of offline extension H142

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List of Acronyms

ASAR Advanced Synthetic Aperture Radar (on Envisat)

ASAR GM ASAR Global Monitoring

ASCAT Advanced Scatterometer

ATBD Algorithm Theoretical Baseline Document

BUFR Binary Universal Form for the Representation of meteorological data

DORIS Doppler Orbitography and Radiopositioning Integrated by Satellite (on Envisat)

ECMWF European Centre for Medium-range Weather Forecasts

ERS European Remote-sensing Satellite (1 and 2)

ESA European Space Agency

EUMETCast EUMETSAT's Broadcast System for Environment Data

EUMETSAT European Organisation for the Exploitation of Meteorological Satellites

FTP File Transfer Protocol

H SAF SAF on Support to Operational Hydrology and Water Management

HTESSEL Hydrology Tiled ECMWF Scheme of Surface Exchanges over Land

LDAS Land Data Assimilation System

Météo France National Meteorological Service of France

Metop Meteorological Operational Platform

NRT Near Real-Time

NWP Numerical Weather Prediction

PRD Product Requirements Document

PUM Product User Manual

PVR Product Validation Report

SAF Satellite Application Facility

SEKF Simplified Extended Kalman Filter

SSM Surface soil moisture

SWI Soil Wetness Index

TU Wien Technische Universität Wien (Vienna University of Technology)

WARP Soil Water Retrieval Package

WARP H WARP Hydrology

WARP NRT WARP Near Real-Time

ZAMG Zentralanstalt für Meteorologie und Geodynamic (National Meteorological Service of Austria)

1. Executive summary

The Algorithm Theoretical Baseline Document (ATBD) provides a detailed description of the algorithm used to produce the H SAF scatterometer root zone soil moisture profile data record product H141 (valid for 1992-2018) and its offline extension H142 (2019-2021). The concept of the H141 production chain is based on scatterometer Surface Soil Moisture (SSM) data assimilation in a dedicated Land Data Assimilation System (LDAS) used to propagate the scatterometer surface soil moisture information in the vertical dimension to the root zone and in the time dimension at the daily time scale. The input information is the surface soil moisture derived from the European Remote Sensing Satellites (ERS) 1/2 Active Microwave Instruments (AMI) for 1992-2006 and the Advanced scatterometer on-board Metop-A (ASCAT-A) for 2007-2018 and Metop-B (ASCAT-B) for 2015-2018, as well as information contained in observations close to the surface (screen level variables; 2-metre temperature and relative humidity). The offline extension of H141 (called H142) includes the assimilation of ASCAT-C in addition to ASCAT-A and ASCAT-B from 2019 to 2021. By the end of the Third Continuous Development and Operations Phase (CDOP-3), H141 and its extension H142 will provide a 30-year scatterometer-derived root-zone SM profile data record (1992-2021).

The H141 production chain is efficient in design since it assimilates scatterometer derived surface soil moisture (SSM) observations into an offline land surface model using a simplified Extended Kalman filter (SEKF). This enables the production of the entire 1992-2018 period at a reasonable computing time (within approximately 4 months). The processing chain is based on the ECMWF land surface model HTESSEL (Hydrology Tiled ECMWF Scheme of Surface Exchanges over Land) constrained by ASCAT-derived SSM assimilation through the SEKF. The land surface model is forced by atmospheric fields provided by the ERA5 state-of-the-art global atmospheric reanalysis [2].

The H141 scatterometer root zone soil wetness index is a multi-year time series (1992-2021), available daily at the global scale and at approximately 10 km resolution. It consists of a root zone soil wetness index profile, provided on four soil layers. It is relevant to hydrological applications, water budget investigations and hydrological trend studies.

An introduction (section 2) to this document is followed by an introduction to the H141 H SAF root zone data record product and its extension H142 (section 3). The production chain is described in section 4 and the output data are illustrated in section 5. A conclusion is given in section 6. Section 7 provides scientific and technical references.

2. Introduction

2.1. Purpose of the document

The Algorithm Theoretical Baseline Document (ATBD) is intended to provide a detailed description of the scientific background and theoretical justification for the algorithms used to produce the root-zone soil wetness index data record (H141) and its offline extension (H142).

2.2. Targeted audience

This document mainly targets:

- Hydrology and water management experts

- Operational hydrology and Numerical Weather Prediction communities
- Users of remotely sensed soil moisture for a range of applications (e.g. climate modelling validation, trend analysis)

2.3. H SAF soil moisture products

In the framework of the H SAF project several soil moisture products, with different timeliness (e.g. near real time products and data records), spatial resolution, format (e.g. time series, swath orbit geometry, global image) or the representation of the water content in various soil layers (e.g. surface, root-zone), are generated on a regular basis and distributed to users. A list of all available soil moisture products, as well as other H SAF products (such as precipitation or snow) can be looked up on the H SAF website (hsaf.meteoam.it). More general information about H SAF can be found in the Appendix. This document describes the production chain of the H141 root zone soil wetness data record product.

3. Introduction to the root-zone soil wetness data record H141

3.1. Principal of the product

The H141 production chain uses an offline sequential Land Data Assimilation System (LDAS) based on an Simplified Extended Kalman Filter (SEKF) method, as in [3]. The SEKF constitutes the central component of the H141 production chain. The HTESSEL Land Surface Model is used to propagate in time and space the soil moisture information through the root zone, accounting for physiographic information (soil texture, orography), meteorological conditions and land surface processes such as soil evaporation and vegetation transpiration [4–6]. H141 is a root zone soil moisture product derived from ERS/SCAT and Metop ASCAT-A/B surface soil moisture (SSM) observations over from 1992 to 2018. Its offline extension H142 assimilates Metop ASCAT-A/B/C from 2019 to 2021 and is updated at a yearly frequency. The retrieval approach for both products relies on an offline, sequential Land Data Assimilation System (LDAS). The ERS1/2 observations are assimilated from 1992 to 2006, the ASCAT-A observations for 2007-2021, ASCAT-B for 2015-2021 and ASCAT-C from 2019-2021. Although the acquisition period of the ERS2 scatterometer extended until September 2011, the ASCAT-A/B data is assimilated instead of ER2 data after 2007 since each ASCAT sensor gives more than twice the coverage (almost daily) of that provided by the ERS scatterometers [7]. The H141 production chain also assimilates screen level parameters close to the surface (2-metre temperature and relative humidity) to ensure consistency of the retrieved Scatterometer root zone and the near surface observed weather conditions. The land surface model is driven by ERA5 atmospheric fields [2]. Figure 3.1 illustrates the H141 LDAS production suite. The H142 production suite is equivalent to H141, except that ASCAT-C is assimilated from 2019 onwards.

3.2. Main characteristics

H141 is produced at a horizontal resolution of about 10km on four vertical layers in the soil: surface to 7 cm, 7 cm to 28 cm, 28 cm to 100 cm, and 100 cm to 289 cm. H141 relies on a data assimilation approach that propagates the information in time and space (on the vertical dimension in the root zone). Therefore, it allows a global update of the root zone soil moisture

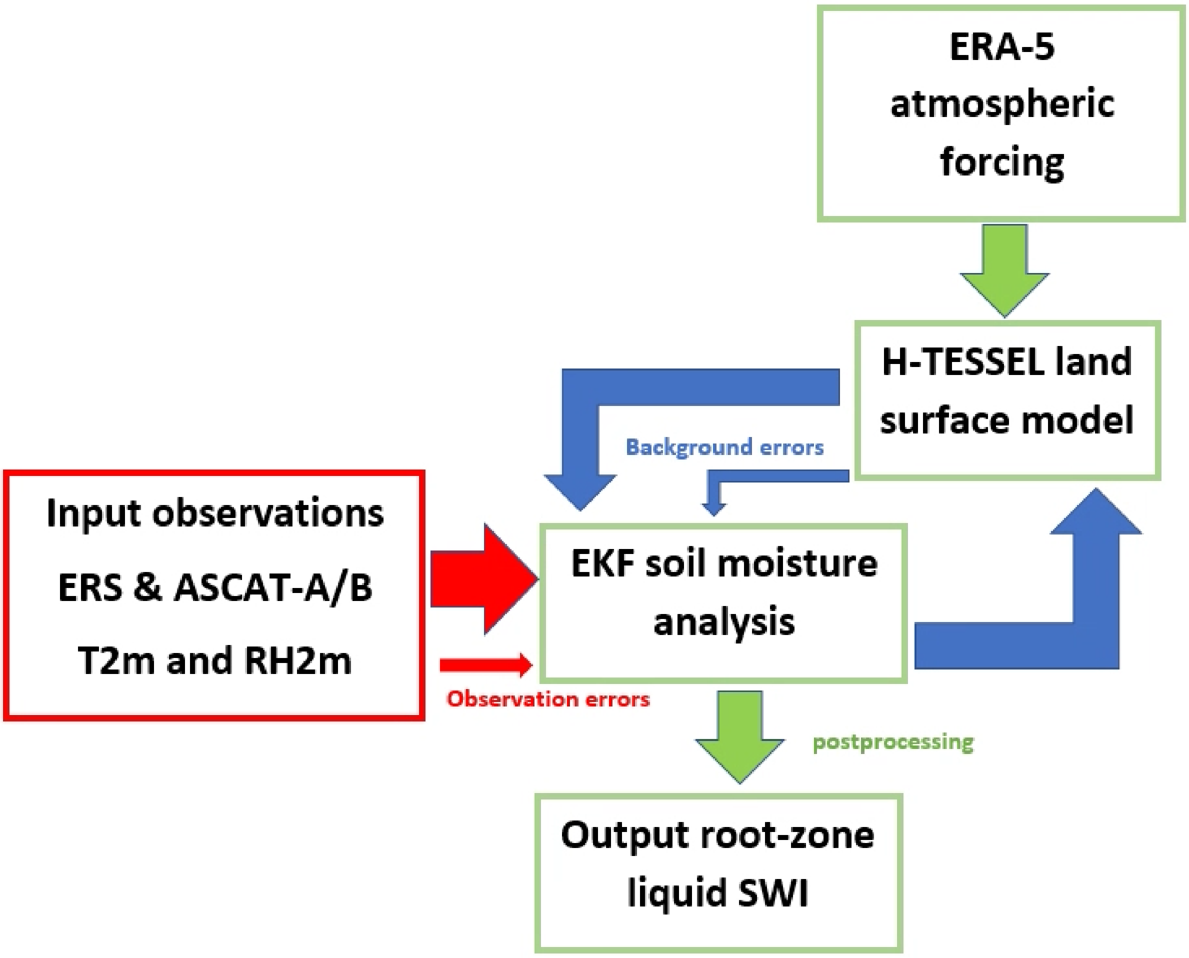


Figure 3.1: Illustration of the H141 root zone soil moisture production chain based on ERS-1/2 and ASCAT-A/B satellite derived surface soil moisture data assimilation.

states using SSM derived from the aforementioned scatterometer products. H141 is a daily product valid at 00UTC. The soil moisture in the model and in the data assimilation process is in volumetric units. Prior to data assimilation, the SSM scatterometer derived observations are rescaled to match the model soil moisture climatology (described in Section 4.1.2) and in the process they are effectively converted to volumetric units. However, the H141 root-zone soil moisture product is expressed as a liquid soil wetness index, with units between 0 (residual soil moisture) and 1 (saturation), representing the lower and upper soil moisture limits. After data assimilation, a post-processing step is required to convert the volumetric soil moisture analysis into the soil wetness index. It is computed using the soil texture (as defined by the FAO/United Nations Educational, Scientific and Cultural Organization (UNESCO) Digital Soil Map of the world [8]), the residual and saturated soil moisture, and the fraction of liquid water content (the fraction of water that is not frozen) on each grid point and each soil layer. Having the units of H141 as a liquid soil wetness index is consistent with all the other ASCAT soil moisture products that are available for the surface (e.g. H14 and H101). Furthermore, it is relevant to various applications and can be combined with different hydrological models (e.g. [9]).

The performance of H141 is estimated by comparing it with in situ observations from 5 in situ networks in the US, Europe and Australia. The NRCS-SCAN network in the US (http://www.wcc.nrcs.usda.gov/scan/, [10]) is the longest running network with observations available from 1997 to 2018. The USCRN network (U.S. Climate Reference Network, [11]) is used over the period 2010 to 2018. The SMOSMANIA (Soil Moisture Observing System Meteorological Automatic Network Integrated Application) network [12, 13] over southwest France has observations from 2007 to 2018. The REMEDHUS network in Spain [14] has data available from 2005 to 2018. Finally, the Oznet network in Australia [15] provides data from 2001 to 2018. Despite this geographical extent limitation, these networks sample a large diversity of soil and vegetation types. They cover most of the soil texture and vegetation types (forest, crops, natural fallow, bare soil) in plains, mountainous, and coastal areas. Following the previous data record (H27/H140) approach, H141 is assessed using the temporal correlation against ground measurements. Additional metrics, including the anomaly correlation coefficient, the root-mean-square error and the bias are also considered. Furthermore, the previous data record product H27/H140 is used as a benchmark to validate the performance of H141 over the period when the data records overlap (1992-2016). Table 3.1 presents the soil wetness index user requirements originally adopted in the H SAF Second Continuous Development and Operations Phase CDOP-2 and also used for the near-real-time (NRT) product (H14) and the H141 data record in the third development phase (CDOP-3). Details and results regarding the validation can be found in the Product Validation Report [16]. The performance of the H142 offline extension is not validated since is assumed to be comparable to H141.

Table 3.1: Performance requirements for products H14 and H141 [CC]

Unit	Threshold	Target	Optimal
Dimensionless	0.5	0.65	0.8

3.3. Product uniqueness and heritage

The H141 data record product supersedes the original H27/H141 data record and includes various modifications, namely increased resolution (16 to 10 km), improved atmospheric forcing

(ERA5 as opposed to ERA-Interim) and the assimilation of ASCAT-B in addition to ASCAT-A observations since 2015. ERA5 has a number of major advantages relative to ERA-Interim, including improved horizontal resolution (31 km instead of 79 km) and an additional decade of model, data assimilation and observing system developments in the ECMWF integrated forecasting system [17]. Furthermore, ERA-Interim will no longer be available after August 2019 and ERA5 forcing will be used for the offline extensions of H141.

Both H141 and H27/H140 assimilate reprocessed ERS1/2 scatterometer observations from 1992-2006. However, H141 covers the period 1992-2018 and assimilates both ASCAT-A from 2007 and ASCAT-B observations from 2015. H142 will then extend the H141 data record from 2019-2021, including the assimilation of ASCAT-C from October 2019 onwards. On the other hand, H27/H140 covers the period 1992-2016 and only assimilates ASCAT-A observations from 2007. The H141 data record product is the only historically consistent scatterometer derived root zone soil wetness index database over the period 1992-2018. The product results from data assimilation which enables the propagation of the surface soil moisture information observed by scatterometers (ERS 1/2 and ASCAT-A/B) to the root zone, taking into account the consistency with ERA5 atmospheric fields used to force the offline LDAS. This makes the H141 product particularly relevant for operational hydrological applications.

The ECMWF H SAF dedicated LDAS has been operational since the First Continuous Development phase (starting in 2012) for the NRT H14 product and the second/third phase for the H27/H140 data record. It is run independently of the ECMWF operational system. The validations of these products have demonstrated that the LDAS is robust, reliable and that it provides high quality root zone soil wetness index fields. H141 is effectively a re-processed and higher resolution version of the H14 root zone product. It is developed using a consistent version of the ECMWF LDAS and using the reprocessed versions of the scatterometer observations from January 1992 until March 2014, then after using NRT observations (see section 4.1 for more details on the input observations). Whereas the production of H14 has been based on the ECMWF/H SAF LDAS system (versions 38R1 in 2012 to 45R1 in 2018) with weakly coupled land-atmosphere DA, the system used to produce H141 was adapted to process a long times series efficiently. Therefore, unlike H14, the H141 LDAS was run offline i.e. the land surface model was not coupled to the atmosphere. H141 therefore used the offline version of the latest ECMWF/H SAF LDAS cycle (46R1) forced by ERA5 atmospheric fields. The main differences between the H14, the H27/and the H141 production chains are summarized in Table 3.2. The offline extension (H142) is equivalent to H141, but covers the period 2019-2021 and includes the assimilation of ASCAT-C from October 2019 onwards.

Table 3.2: Differences between H14 (near-real-time), H27/H140 (data records) and H141 (data record) production chains. The * superscript implies that the observations were reprocessed from January 1992 to March 2014. N.A. stands for "not applicable".

Product	H14 NRT	H27/H140 data record	H141 data record
Period	2012-present	1992-2016	1992-2018
SM observations	ASCAT-A/B SSM	ERS 1/2* (1992-2006) and ASCAT-A* (2007-2016)	ERS 1/2* (1992-2006) and ASCAT-A/B* (2007-2018)
DA system	Regular updates of LDAS (38R1-45R1)	Fixed LDAS cycle 41R1 (43R3) for H27 (H140)	Fixed LDAS cycle 46R1
Atmos. forcing	N.A.	ERA-Interim	ERA5
Resolution	25 km	16 km	10 km

4. Production chain

The main components of the H141 production as presented in Figure 3.1 are detailed hereafter. They include the input data and pre-processing, the HTESSEL land surface model and the SEKF data assimilation system.

4.1. Input data and reprocessing

4.1.1. Remotely sensed soil moisture

Scatterometer surface soil moisture products from ERS-1/2 (from 1992 to 2006) Active Microwave Instruments (AMI), the ASCAT-A from 2007 to 2018 and ASCAT-B from 2015-2018 are used as the main input of the H141 production chain. ASCAT-A/B and (2019-2021) and ASCAT-C (October 2019 to 2021) are the main inputs to the offline extension H142. Table 4.1 below gives the details on the scatterometer SSM products used as input of the H141 and H142 production suites. As shown in Table 4.1, there is no overlap between ERS1/2 and ASCAT-A observations used to produce H141. The ERS1/2 and ASCAT-A observations are reprocessed from January 1992 to March 2014. From April 2014 the operational version of ASCAT-A was assimilated since the reprocessed observations were unavailable. The ASCAT-B observations were assimilated together with ASCAT-A from 2015. Figure 4.1 shows the longitudinal monthly means of SSM from ERS-1/2 AMI (top) and ASCAT on board Metop-A (bottom). It illustrates the long time series of scatterometer soil moisture used as input for H141. The addition of ASCAT-B from 2015-2018 (not shown) approximately doubles the total number of observations and significantly increases the global coverage in mid-latitudes ([18] gives details). ASCAT-C further increases the observation count from October 2019. ASCAT-A is currently in a drift orbit, but it is foreseen that it will remain operational until 2021.

The ERS and ASCAT-A/B sensors operate at similar frequencies (5.3 GHz C-band) and share a similar design. ERS AMI has three antennas (fore- mid-, and aft-beam) only on one side of the instrument whilst ASCAT-A/B has them on both sides, which more than doubles the area covered per swath. ERS AMI data coverage is variable spatially and temporally because of conflicting operations with the synthetic aperture radar (SAR) mode of the instrument. In addition, due to the failure of the gyroscope of ERS-2, the distribution of scatterometer data was temporarily discontinued from January 2001 [19] whereas in June 2003 its tape drive failed (as seen in Figure 4.1). Complete failure of ERS-1 and ERS-2 occurred in 2000 and 2011, respectively. Estimates of soil moisture are computed using the WARP 5.2 change detection method [20,21], which provides a soil moisture fraction between residual soil moisture (0%) and full saturation (100%) for the top few centimetres of the soil. Both ascending and descending overpasses were used.

The ASCAT-A reprocessed dataset has been chosen for its consistency over the period when it is assimilated (January 2007 - March 2014). Compared to its operational counterpart, it has a better match with in situ measurements of soil moisture, as illustrated by Figure 4.2. Figure 4.2 illustrates correlations (left panel) and anomaly correlations (right panel) between the ASCAT-A operational product and in situ measurements of surface soil moisture against correlations between the ASCAT-A reprocessed product and the same in situ observations from 2010-2013. For the calculation of the anomaly correlations, the difference to the mean is calculate using a sliding window of 5 weeks. The in situ observations come from the USCRN network (U.S. [11]). Symbols above the diagonal indicate that the ASCAT-A reprocessed dataset better matches

Table 4.1: H141 (1992-2018) and H142 (2019-2021) input scatterometer SSM products.

	Scaterrometer SSM product used in H141 data record		
Period	Sensor	Producer	Reference
04-2014 to 12-2021	ASCAT-A (03/2014 to 12/2021), ASCAT-B (01/2015 to 12/2021) and ASCAT-C (10/2019 to 12/2021) 25 km sampling	EUMETSAT CAF	ASCSMO02: ASCAT-A/B/C 25 km swath grid product distributed by CAF. (https://vnavigator.eumetsat.int/product/EO:EUM:DAT:METOP:SOMO25). Equivalent to H SAF level 2 surface soil moisture products H102 (Metop-A 25 km sampling), H103 (Metop-B 25 km sampling) and H105 (Metop-C 25 km sampling).
01-2007 to 03-2014	ASCAT-A 25 km sampling	TU Wien	H107: H SAF soil moisture data record reprocessed level 2 surface soil moisture.
01-1992 to 12-2006	ERS 1/2 AMI 50 km sampling	TU Wien	ERS-1/2 AMI WARP 5.5 R1.1: ERS-1/2 AMI 50km Soil moisture time series product. Produced as part of the Scirroco project (https://earth.esa.int/documents/) 700255/2925769/SCI-PRE-2015-0001-v-01-SM_reprocessing_TUW.pdf) using the Water Retrieval Package (WARP) version 5.5.

the in situ measurements. The figure shows that the reprocessed version of ASCAT-A SSM is in better agreement with in situ data than the operational version that was assimilated in the H14 NRT product. Therefore the reprocessed observation input used in H141 has an improved quality compared to that of H14.

A quality control is applied to filter input ERS 1/2 and ASCAT-A/B SSM observations so that only observations with a noise level lower than 15% are used for H141. The quality control also rejects ERS 1/2 and ASCAT-A/B SSM observation for pixels with a water fraction larger than 15% and with a topographic complexity larger than 20%, as well as observations in frozen soil and/or snow covered surface conditions. When no observations are assimilated, the root zone soil moisture entirely relies on the HTESSEL land surface model, which ensures physically based soil moisture evolution when there are gaps in the scatterometer observations.

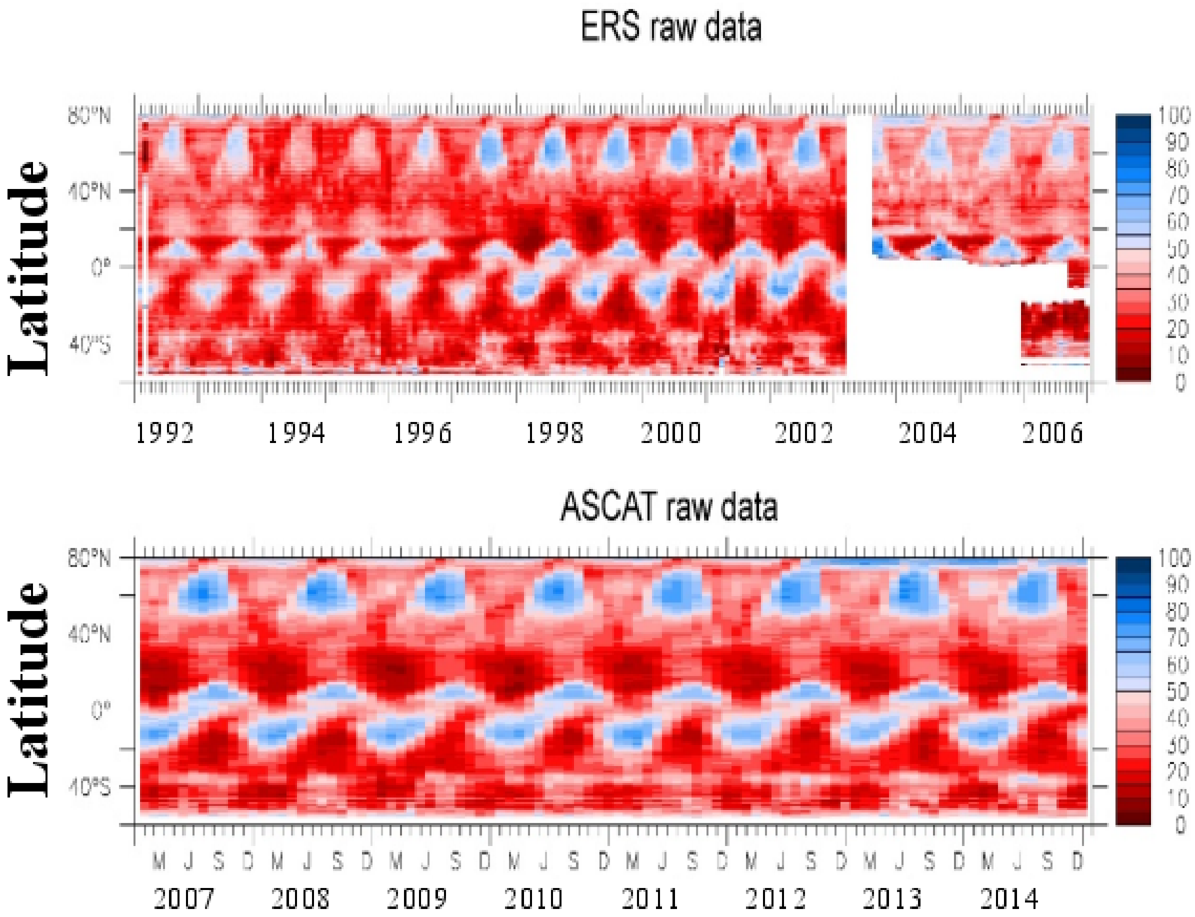


Figure 4.1: H141 ERS1/2 and ASCAT-A input scatterometer SSM products. The original Figure can be found in the H27/H140 ATBD [1].

4.1.2. Rescaling

In the context of the assimilation of soil moisture data, the considered observations need to be re-scaled to be consistent with the model climatology [22–24]. Each soil moisture data set is characterized by its specific mean value, variability and dynamical range. The HTESSEL land

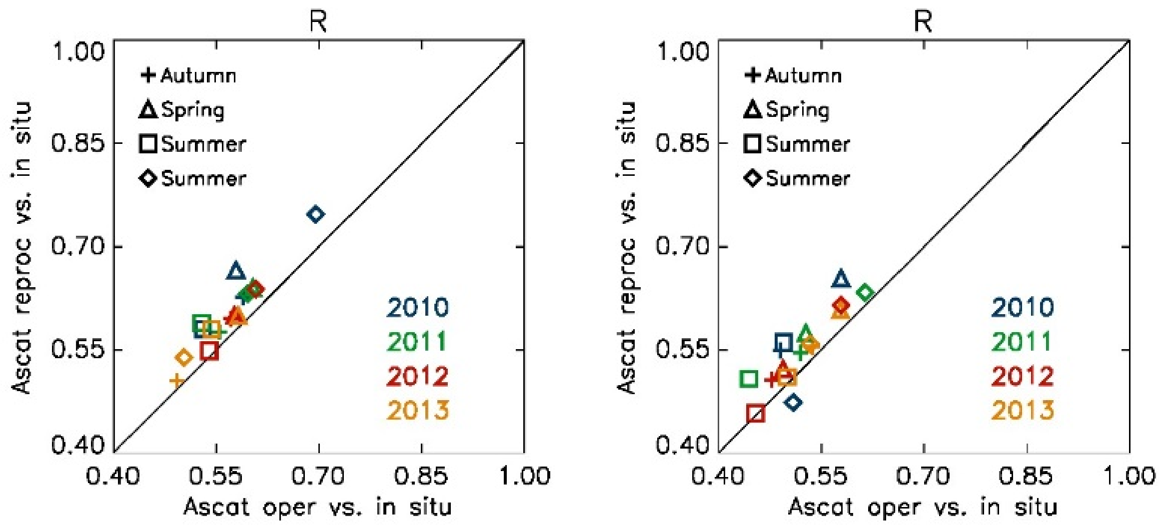


Figure 4.2: Correlations (left) and anomaly correlations (right) between ASCAT-A operational product and in situ measurements of surface soil moisture against correlations between ASCAT-A reprocessed product and the same in situ measurements. All seasons and years over 2010-2013 are represented and the in situ measurements belong to the USCRN network (114 stations) spanning much of the USA.

surface model has its own soil moisture climatology with a specific dynamical range controlled by the values at the wilting point and field capacity (functions of soil textural types). The ERS1/2 and ASCAT-A/B SSM products (index) have to be transformed into model equivalent volumetric SSM. The approach described in [22] (using a simplified form of a Cumulative Distribution Function, CDF) is used here. It is a linear rescaling technique designed to match the mean and variance of the model and observations. The two parameters of the linear relationship, the intercept A and the slope B, vary spatially but are constant in time:

$$\begin{aligned} A &= \overline{\theta}_m - B \times \overline{\theta}_o \\ B &= \frac{\sigma_m}{\sigma_o}, \end{aligned} \tag{1}$$

where $\overline{\theta}_m$ and $\overline{\theta}_o$ stand for the means of model and observation surface soil moisture, respectively, while σ_m and σ_o represent the standard deviations of model and observations, respectively. The rescaling parameters are derived for each point individually using the modelled and observed soil moisture from 2007 to 2013. [25, 26] accounted for the seasonal variability in the model by varying the rescaling parameters in the bias correction according to the month of the year. In line with these studies, the A and B parameters were derived on a seasonal basis by using a three-month moving window over 2007 to 2013 after screening of the ASCAT-A/B SSM data using (1) their own quality flags and (2) the presence of snow and soil temperature below 0°C. Figure 4.3 illustrates A (left) and B (right) parameters for January (top) and June (bottom). The snow line is visible in the Northern Hemisphere. These maps show that the ERS1/2 and ASCAT-A/B SSM observations are not used over tropical forest and they are not used in frozen or in snow covered conditions, nor in complex topography areas or where large water bodies are expected to contaminate the signal (see previous section). In this case the root-zone soil moisture will come from the land surface model, thereby ensuring physically based soil moisture evolution. Figure 4.4 illustrates the impact of the linear rescaling of ASCAT-A satellite derived surface soil moisture for January to March 2007 for one location in Southwestern France (X=1.17E,Y=43.82N).

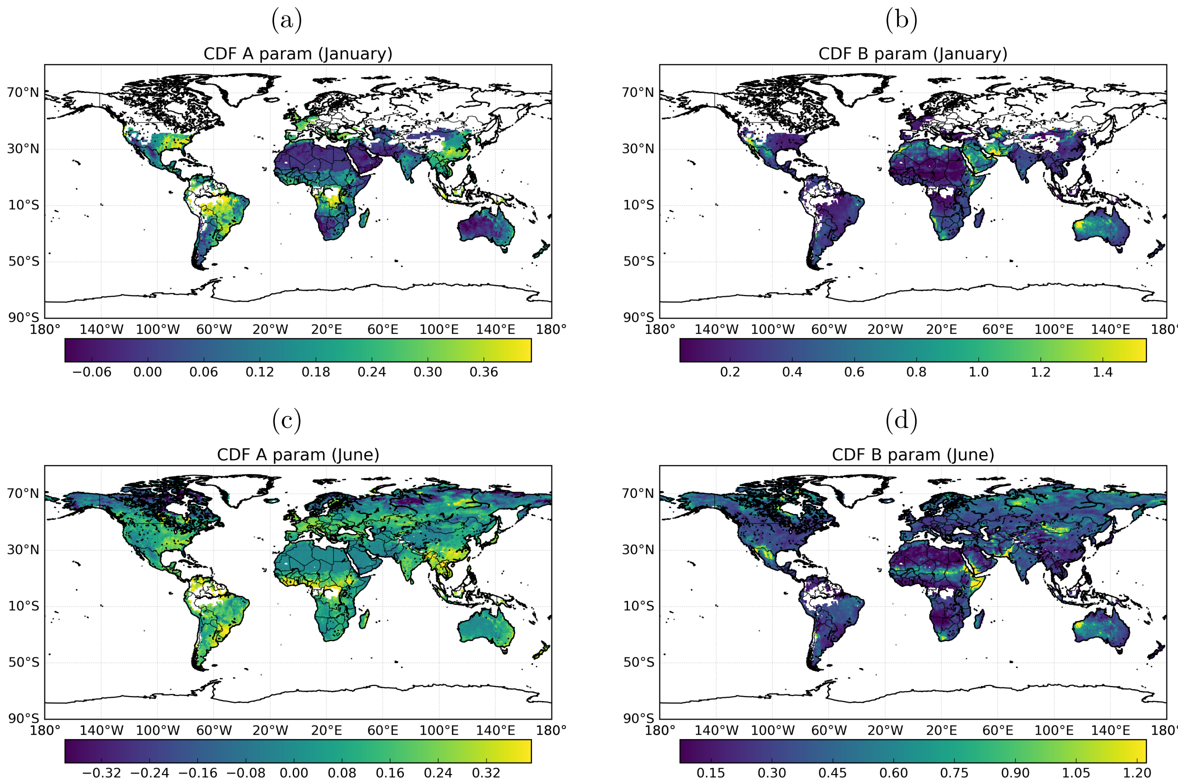


Figure 4.3: Linear rescaling parameters (a) A for January, (b) B for January, (c) A for June, (d) B for June.

4.1.3. Screen Level Variables (2-metre temperature and relative humidity)

The H141 production chain also assimilates screen level variables (2-metre temperature and relative humidity). Most current operational soil moisture analysis systems rely on analysed screen-level variables; 2m temperature and relative humidity [3,27]. In the absence of a near-real-time global network for providing soil moisture information, screen level data is the only source of information that has been continuously available in real time for NWP soil moisture analysis systems. As shown by [28] and [29], screen-level parameters provide indirect, but relevant, information to analyse soil moisture. Analysed fields of 2-metre temperature (T2M) and 2-metre relative humidity (RH2M) from the ERA5 reanalysis [2, 17] are assimilated in the H141 production chain by the SEKF. They were obtained in ERA5 using an optimal interpolation method leading to a global coverage of the two variables. Similarly, T2m and RH2m fields are also assimilated in the NRT H14 product.

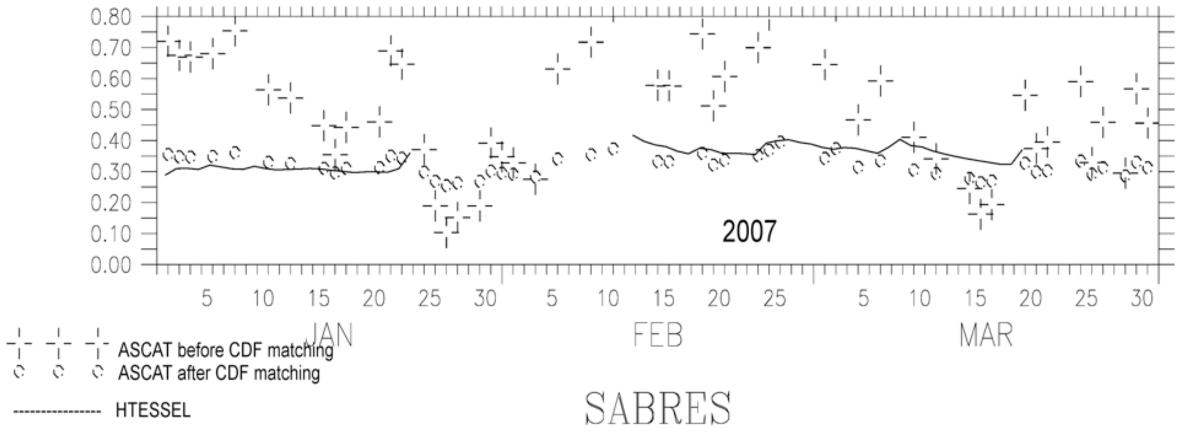


Figure 4.4: Time series of ASCAT-A observations in January-March 2007 before and after CDF matching at the Sabres station in southwest France (1.17°E, 43.82°N). The CDF matched ASCAT observations are assimilated in H141.

4.2. The HTESSEL land surface model

In the H141 production chain, the temporal and vertical propagation of soil moisture from the surface soil towards the root zone is driven by the HTESSEL land surface model [4–6]. The HTESSEL formulation of the soil hydrological conductivity and diffusivity accounts for spatial variability according to a global soil textural map [8]. A monthly leaf area index (LAI) climatology is used based on a MODIS satellite product as described in [30]. Surface runoff is based on the variable infiltration capacity. The soil heat budget follows a Fourier diffusion law, modified to take into account soil water freezing/melting according to [31]. The energy equation is solved with a net ground heat flux as the top boundary condition and a zero flux at the bottom. The water balance at the surface (i.e., the change in water storage of the soil moisture, interception reservoir, and accumulated snowpack) is computed as the difference between the precipitation and (i) the evaporation of soil, vegetation, and interception water and (ii) surface and subsurface runoff. First precipitation is collected in the interception reservoir until it saturated. Then, excess precipitation is partitioned between surface runoff and infiltration into the soil column. Bare ground evaporation over dry land uses a lower stress threshold than for the vegetation, allowing a higher evaporation [32]. This is in agreement with the modelled findings of [28] and results in more realistic soil moisture for dry land [33].

4.3. Extended Kalman filter

A point-wise SEKF is used to assimilate scatterometer surface soil moisture to produce the root zone soil moisture, which is converted afterwards into the H141 soil wetness index. The SEKF constitutes the core of the H141 production chain. On each grid point the analysis update equation of the SEKF is expressed as:

$$\mathbf{x}^a(t_0) = \mathbf{x}^f(t_0) + \mathbf{B}_i\mathbf{H}_i^T(\mathbf{H}_i\mathbf{B}_i\mathbf{H}_i^T + \mathbf{R}_i)^{-1}(\mathbf{y}^o(t_i) - h(\mathbf{x}^f(t_i))), \quad (2)$$

where $\mathbf{x}$ is the control state vector which is the vertical soil moisture profile for the n analysed layers of the land surface model. The number of observations assimilated has dimension p. $\mathbf{B}$ is the background error covariance matrix (of dimension n times n), $\mathbf{R}$ is the observation error covariance matrix (of dimension p times p). The "a", "f" and "o" superscripts denote analysis, forecast and observation, respectively. Transpose matrices are indicated by the superscript T. The analysis is performed at the start of the window (t_0) at 00 UTC and the information from the observations is implicitly propagated from the times of the observations (t_i) in the 24 hour window to the analysis time via the observation operator Jacobians (equation (4.3.1) in Section 3) and the SEKF equation (2). The observation operator is denoted by h, which transforms the model control variables into the observation space at the observation time (t_i). In the H141 production chain, n=3, with the top three layers being analysed. $\mathbf{y}^o$ is the observation vector which contains p observations of 2m temperature, 2m relative humidity and surface soil moisture scatterometer observations available within the data assimilation window. The screen-level observations and scatterometer-derived SSM observations are assimilated at either 00, 06, 12 or 18 UTC (as detailed in section 4.1). The observation operator h allows the computation of the model counterpart of the observations. The linearized observation operator $\mathbf{H}$ is a matrix of dimension n times p and each element in $\mathbf{H}$ is a Jacobian representing the tangents of the observation operator at the observation times.

4.3.1. Jacobian matrix

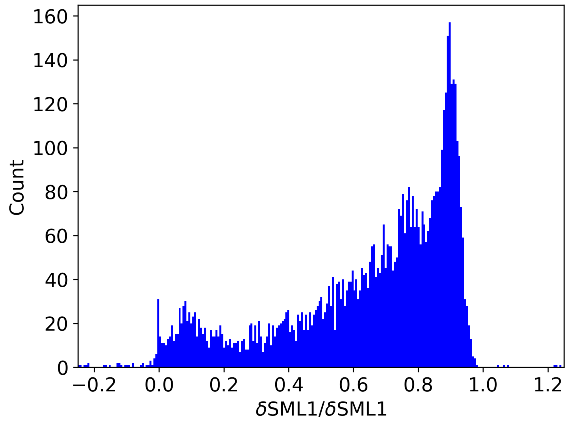
The elements of the Jacobian matrix $\mathbf{H}$ are estimated by finite differences, by individually perturbing each prognostic variable j of the initial control vector $\mathbf{x}^b(t_0)$ by a small amount $\delta\mathbf{x}_j$ to get for each integration a column of the matrix $\mathbf{H}$:

$$\mathbf{H}_{ij} = \frac{y_i(\mathbf{x}(t_0) + \delta\mathbf{x}_j) - y_i(\mathbf{x}(t_0))}{\delta\mathbf{x}_j}, \tag{3}$$

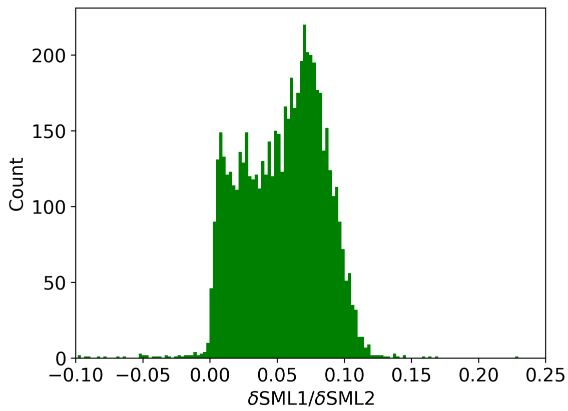
where $\mathbf{y}_i = h(\mathbf{x}_i)$ is the model predicted value of the observations at time t_i. As in [34] and [3] a 0.01 $\mathrm{m^3m^{-3}}$ soil moisture perturbation is used in HTESSEL for the H141 production chain as the linearity assumption in the finite difference approximation of the Jacobians was shown to be accurate for perturbations of this size. In this configuration, for every 1-day analysis cycle, the model trajectory is run four times to compute the Jacobian matrix elements of Equation (3); one unperturbed model trajectory (over the 24-hour assimilation window) and three trajectories from perturbing the soil moisture initial conditions of the first, second and third layers. Note that the Jacobians for the 4th layer are not calculated since it is not analysed.

The elements of the Jacobian matrix are governed by the physics of the model. Their examination is important to understand the data assimilation system performances [35]. As illustrated by the histograms of Figure 4.5 for one site located in southwest France (corresponding to the Saint Felix station of the SMOSMANIA network, 43.44°N/1.88°E), the sensitivity of SSM to changes in soil moisture of the first layer of soil is higher than that of the second and third layers of soil (Figure 4.5 a, c and d, respectively), revealing that the assimilation system will be more effective in modifying soil moisture from the first layer. This sensitivity is reduced close to the field capacity threshold (as illustrated by Figure 4.5b).

(a) $\frac{\delta \mathrm{SML1}}{\delta \mathrm{SML1}}$ histogram



(b) $\frac{\delta \mathrm{SML1}}{\delta \mathrm{SML2}}$ histogram



(c) $\frac{\delta \mathrm{SML1}}{\delta \mathrm{SML3}}$ histogram

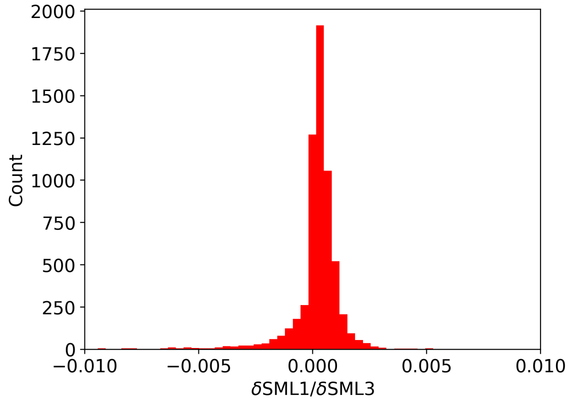


Figure 4.5: Illustration of Jacobians for one site located in the France (corresponding to the station Saint Felix of the SMOSMANIA network, 43.44°N/1.88°E), The histograms of the Jacobians of SSM to perturbations in soil moisture layers 1, 2 and 3 are shown in Figures (a), (c) and (d) respectively. The scatter plot (b) shows the SSM Jacobians for the first layer against the soil moisture at the same points with the wilting point (red line) and field capacity (black line).

4.3.2. Error specifications

The description of the error matrices is a key aspect of data assimilation [36,37]. The correction of the system state depends on the background and observation error specifications. The soil moisture component of the observation-error covariance matrix **R** varies both in time and space, as the ERS1/2 and ASCAT-A/B noise level information [22] provide the observation errors. Observation error covariances for RH2M and T2M are set to 4% and 2 Kelvin, respectively.

The background error covariance matrix **B** is a diagonal matrix. Recall that the data assimilation is performed in volumetric units, which is consistent with the HTESSEL model. Following [38], the soil moisture background errors are assumed to be proportional to the volumetric dynamic range. This is defined as the difference between the volumetric field capacity and the wilting point. Above the field capacity, gravitational drainage will rapidly remove soil moisture from the soil, whilst below the wilting point, transpiration will cease. It is worth noting that the soil moisture can temporarily exceed (fall below) the field capacity (wilting point) during prolonged wet (dry) conditions. Therefore the residual soil moisture (lower soil moisture limit) is less than the wilting point and the saturation (upper soil moisture limit) is higher than the field capacity. The dynamic range depends on the soil textural type, with clayey soils having a larger dynamic range than sandy soils. The background error standard deviations are defined as 5% of the volumetric dynamic range.

4.3.3. Data assimilation window length and cycling

The H141 production chain relies on a 24h data assimilation window, covering 00 UTC to 24 UTC daily. The SSM scatterometer observations have a temporal resolution between 1 and 3 days but may occur at any points in the 24 hour window depending on their location. The observations are assumed to occur at the nearest 6-hour time interval. Analysed screen level variables (two-metre temperature and relative humidity) available at 06:00, 12:00 and 18:00UTC, and scatterometer SSM observations available at 00:00 (+/-3h), 06:00(+/-3h), 12:00 (+/-3h) and 18:00 (+/-3h) UTC are assimilated. The increments are applied at the beginning of the 24-hour data assimilation window, as in the equivalent simplified 2D-Var described in [39]. So, for each 24-hour analysis cycle, the H141 production suite runs five trajectories of HTESSEL:

- The first trajectory provides the model background;
- The second, third and fourth trajectories are produced by perturbing the soil moisture initial conditions of the first, second and third layer, respectively;
- The fifth trajectory is produced with the analysis increments applied at the beginning of the 24-hour window. It is the analysed trajectory. Its 24 h window length provides the initial conditions of the next data assimilation window.

5. Output data

5.1. H141 production chain output data

The H141 output data are provided at approximately 10 km resolution in two different formats in order to cater for the needs of different users. The model and data assimilation are performed on a cubic octahedral reduced Gaussian grid, which has approximately equidistant grid points between the equator and the poles. For each date a single GRIB file is provided of the soil moisture analysis in the original reduced Gaussian grid format, giving four fields of global soil wetness index (one for each soil layer). Additionally, the same fields are provided as a single netCDF file in a regular lat/lon format (created by interpolating the reduced Gaussian grid into a regular lat/lon grid). A more detailed description of the data format and structure can be found in the H141 Product User Manual [40].

5.2. Example of H141 analysis increments and output data

This section illustrates the H141 increments and output data. Figure 5.1(a) and 5.1(b) represent daily averaged analysis increments over the first meter of soil expressed in mm (i.e., impact of assimilating satellite derived surface soil moisture and screen level variables in the system) for January and June 2009 respectively. From Figure 5.1(a) one can see the snow line in the North hemisphere as no data are assimilated in presence of snow. From Figure 5.1(b), it is possible to see that for the month of June 2009, the analysis added water over the Sahel in Africa, northern India, eastern Europe into the Middle East, Northern Australia and central parts of North America. It removed water over western Europe, southeast Asia and parts of Argentina, among other areas.

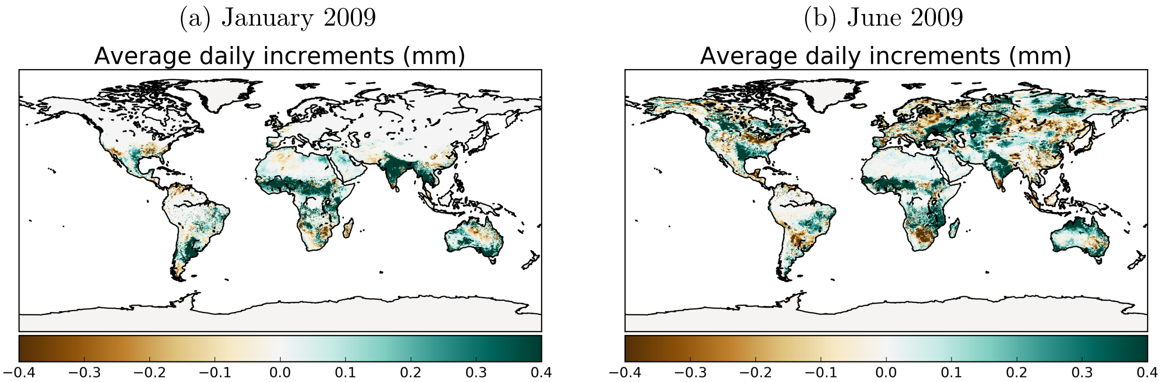


Figure 5.1: Average daily H141 analysis increments for the first metre of soil for (a) January 2009 and (b) June 2009. Brown (green) colours indicate that the analysis removed (added) water. The legend is expressed in mm per day.

Figure 5.2 shows a time series plot of H141 averaged over Europe from 2001-2010. The exceptionally warm and dry summers of 2003 and 2006 are reflected by anomalously low root-zone SWI values. Figures 5.3 and 5.4 are H141 previews for 2 days; 01 January 2011 and 01 June 2011 respectively. The four layers of H141 are represented (0-7 cm, 7-28 cm, 28-100 cm and 100-289 cm from top to bottom). Note that only the first three layers are analysed. As H141 represents the liquid part of the surface and root zone soil wetness index, one may notice that in winter (Figure 5.3) the Northern areas (affected by snow and cold temperatures) share the same colour code as dry areas (e.g. the Sahara desert in Africa).

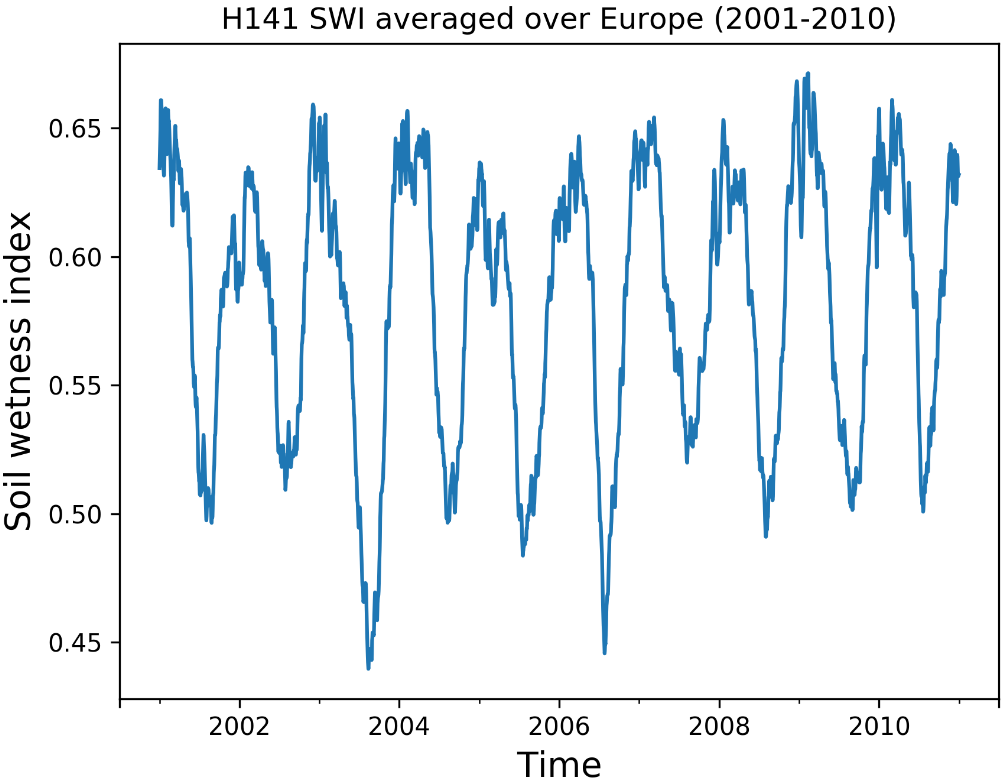


Figure 5.2: H141 root-zone SWI time series for 2001-2010.

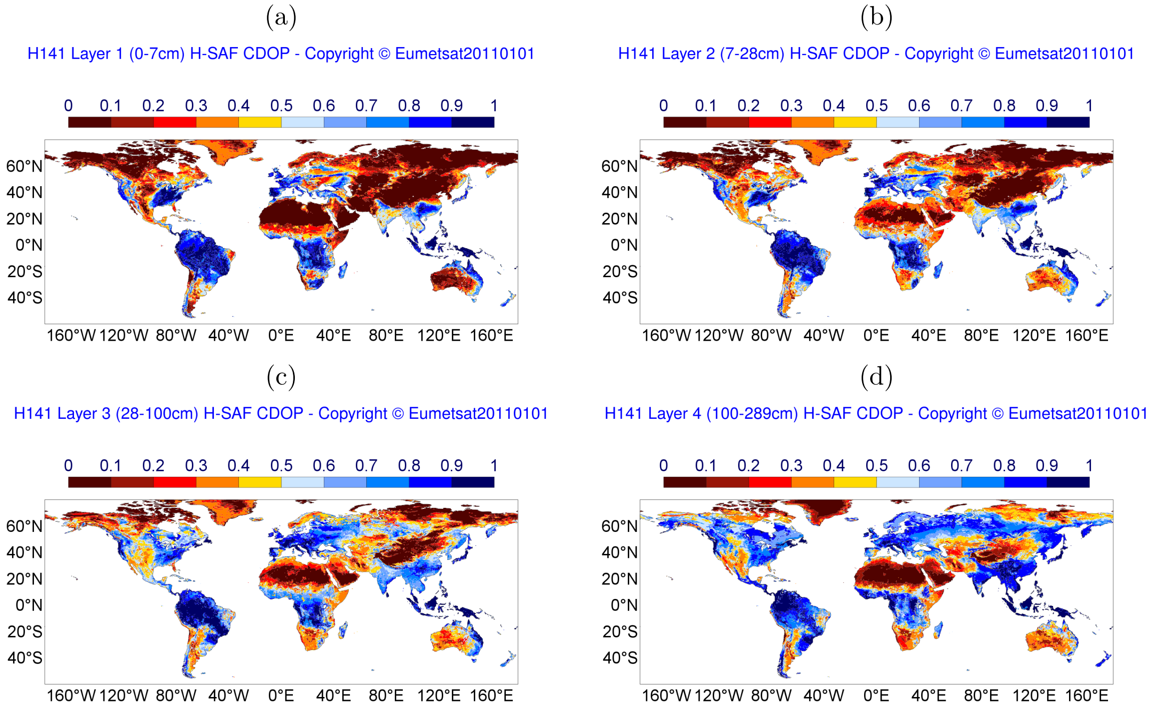


Figure 5.3: H141 previews for 01 January 2011 for the 4 layers of soil: (a) 0-7 cm, (b) 7-28 cm, (c) 28-100 cm and (d) 100-289 cm.

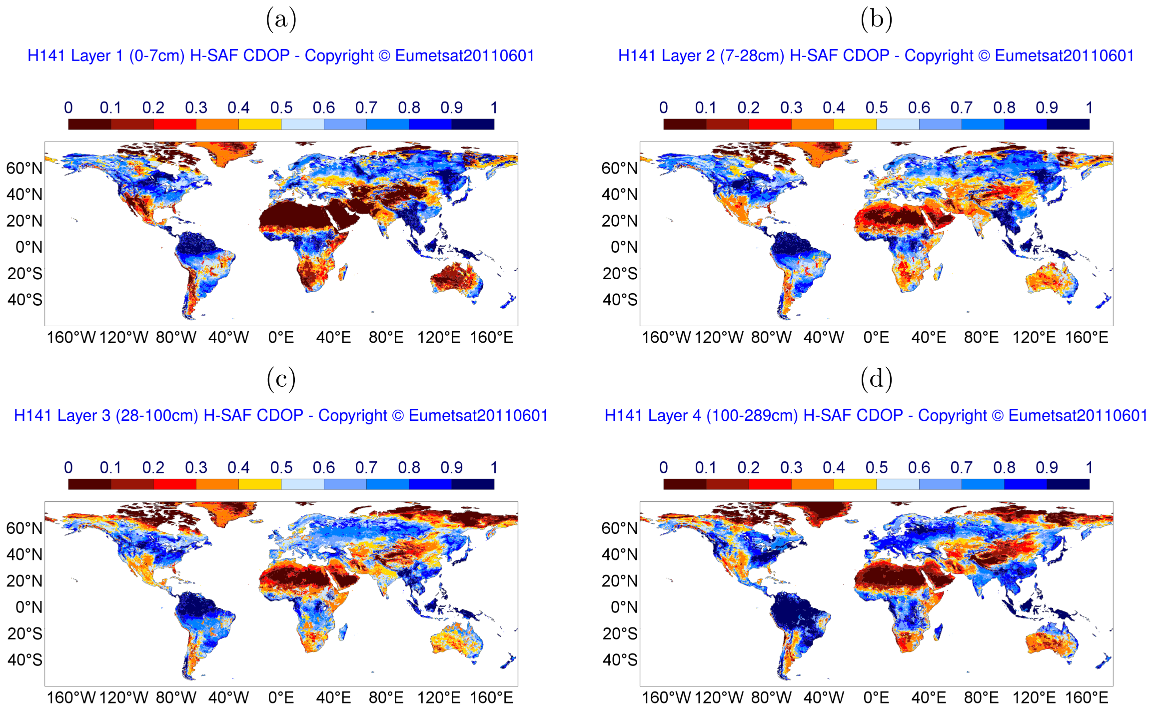


Figure 5.4: Same as Figure 5.3 but for 01 June 2011.

6. Conclusion

The H141 data record product consists of a unique historically consistent scatterometer derived root zone soil wetness index database over the period 1992-2018. Its offline extension H142 will extend the H141 data record to the end of the CDOP-3 (2019-2021). The product results from data assimilation which enables the propagation of the surface soil moisture information observed by scatterometers (ERS 1/2 and ASCAT-A/B/C) to the root zone, taking into account the consistency with ERA5 atmospheric fields used to force the offline LDAS. It improves on the original root-zone data record product (H27/H140) through superior atmospheric forcing (ERA5 instead of ERA-interim), increased resolution (10 km instead of 25 km) and the assimilation of ASCAT-B and ASCAT-C from 2015 and 2019 respectively. The re-processed scatterometer observations from January 1992 to March 2014 used in H141 are more accurate than their operational counterpart. H141 is expected to provide benefits for a range of research activities, including hydrological applications, water budget investigations and hydrological trend studies.

The 10 km resolution H141 product is provided daily as a soil wetness index across the four root-zone layers. More information about the output format and visualizations of H141 can be found in the H141 product user manual [40]. A comprehensive validation against in situ measurements can be found in the product validation report [16].

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Appendices

A. Introduction to H SAF

H SAF is part of the distributed application ground segment of the "European Organization for the Exploitation of Meteorological Satellites (EUMETSAT)". The application ground segment consists of a Central Application Facilities located at EUMETSAT Headquarters, and a network of eight "Satellite Application Facilities (SAFs)", located and managed by EUMETSAT Member States and dedicated to development and operational activities to provide satellite-derived data to support specific user communities (see Figure A.1):

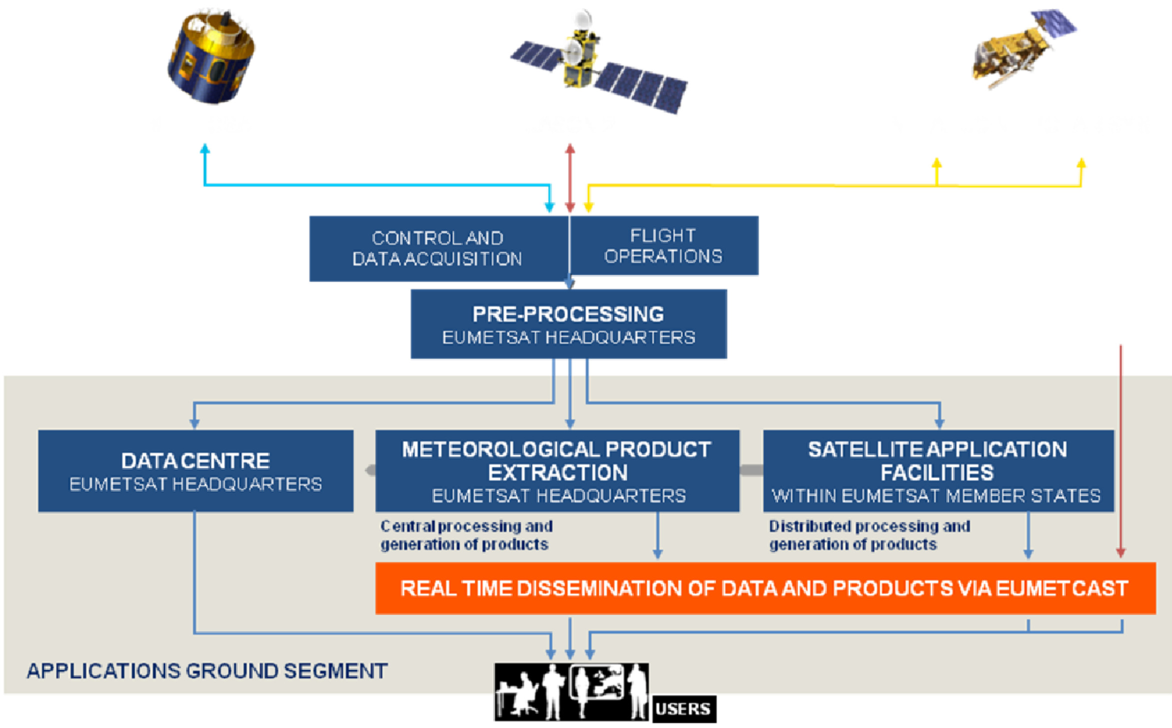

Figure A.1: Conceptual scheme of the EUMETSAT Application Ground Segment.

Figure A.2 here following depicts the composition of the EUMETSAT SAF network, with the indication of each SAF's specific theme and Leading Entity.

B. Purpose of the H SAF

The main objectives of H SAF are:

a) to provide new satellite-derived products from existing and future satellites with sufficient time and space resolution to satisfy the needs of operational hydrology, by generating, centralizing, archiving and disseminating the identified products:

- precipitation (liquid, solid, rate, accumulated);
- soil moisture (at large-scale, at local-scale, at surface, in the roots region);

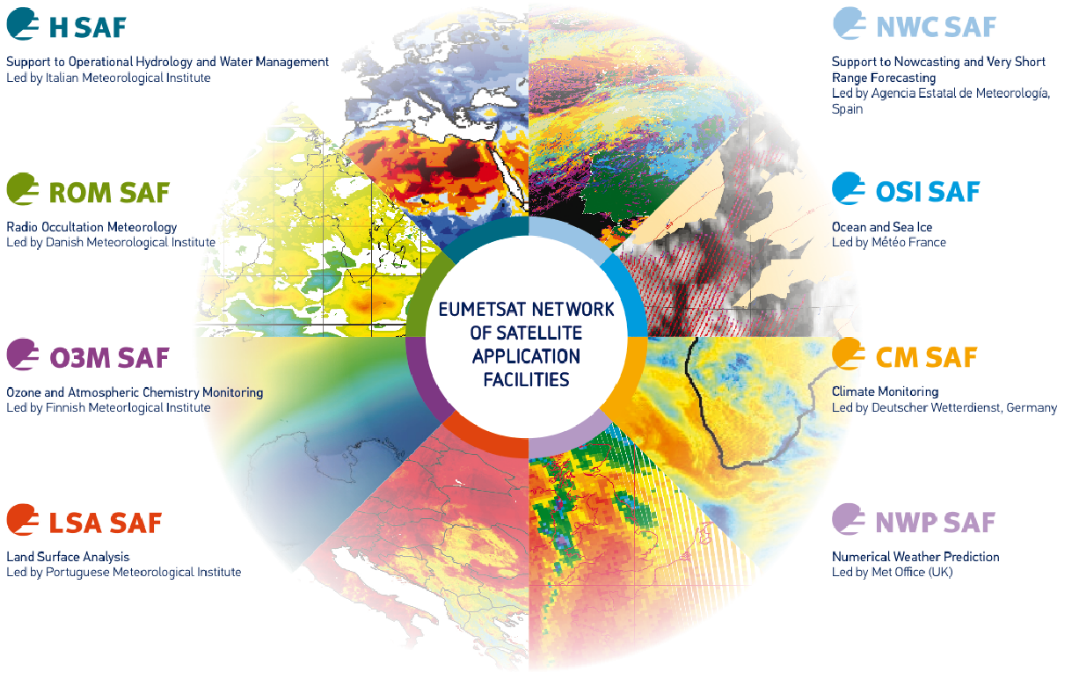

Figure A.2: Current composition of the EUMETSAT SAF Network.

- snow parameters (detection, cover, melting conditions, water equivalent);

b) to perform independent validation of the usefulness of the products for fighting against floods, landslides, avalanches, and evaluating water resources; the activity includes:

- downscaling/upscaling modelling from observed/predicted fields to basin level;
- fusion of satellite-derived measurements with data from radar and raingauge networks;
- assimilation of satellite-derived products in hydrological models;
- assessment of the impact of the new satellite-derived products on hydrological applications.

C. Products / Deliveries of the H SAF

For the full list of the Operational products delivered by H SAF, and for details on their characteristics, please see H SAF website hsaf.meteoam.it. All products are available via EUMETSAT data delivery service (EUMETCast[1]), or via ftp download; they are also published in the H SAF website[2].

All intellectual property rights of the H SAF products belong to EUMETSAT. The use of these products is granted to every interested user, free of charge. If you wish to use these products, EUMETSAT's copyright credit must be shown by displaying the words "copyright (year) EUMETSAT" on each of the products used.

[1] http://www.eumetsat.int/website/home/Data/DataDelivery/EUMETCast/index.html
[2] http://hsaf.meteoam.it

D. System Overview

H SAF is lead by the Italian Air Force Meteorological Service (ITAF MET) and carried on by a consortium of 21 members from 11 countries (see website: hsaf.meteoam.it for details)

Following major areas can be distinguished within the H SAF system context:

- Product generation area
- Central Services area (for data archiving, dissemination, catalogue and any other centralized services)
- Validation services area which includes Quality Monitoring/Assessment and Hydrological Impact Validation.

Products generation area is composed of 5 processing centres physically deployed in 5 different countries; these are:

- for precipitation products: ITAF CNMCA (Italy)
- for soil moisture products: ZAMG (Austria), ECMWF (UK)
- for snow products: TSMS (Turkey), FMI (Finland)

Central area provides systems for archiving and dissemination; located at ITAF CNMCA (Italy), it is interfaced with the production area through a front-end, in charge of product collecting. A central archive is aimed to the maintenance of the H SAF products; it is also located at ITAF CNMCA.

Validation services provided by H SAF consists of:

- Hydrovalidation of the products using models (hydrological impact assessment);
- Product validation (Quality Assessment and Monitoring).

Both services are based on country-specific activities such as impact studies (for hydrological study) or product validation and value assessment. Hydrovalidation service is coordinated by IMWM (Poland), whilst Quality Assessment and Monitoring service is coordinated by DPC (Italy): The Services activities are performed by experts from the national meteorological and hydrological Institutes of Austria, Belgium, Bulgaria, Finland, France, Germany, Hungary, Italy, Poland, Slovakia, Turkey, and from ECMWF.