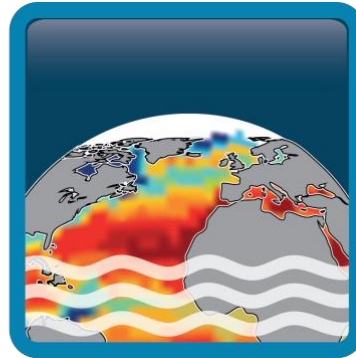


# Climate Change Initiative+ (CCI+) Phase 1

## Sea Surface Salinity



### [D1.2] Product Specification Document (PSD)

**Customer: ESA**

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**National Oceanography Centre**  
NATURAL ENVIRONMENT RESEARCH COUNCIL







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## Amendment Record Sheet

	Document Change Record	
Date / Issue	Description	Section / Page
01/02/19 v1r4	Deliver to ESA	New document
23/04/19 v1r5	Revision following ESA comments	N/A
24/04/19 v1r6	New document template	2.2
05/08/19 v1r7	Updated attribute list, data access information	2.3 & 2.4
15-09-2021 / v2.0	Update document template Updated with final CRDP	All

## Table of Contents

<b>Signatures .....</b>	<b>iv</b>
<b>Amendment Record Sheet .....</b>	<b>vi</b>
<b>Table of Contents .....</b>	<b>vii</b>
<b>List of figures .....</b>	<b>viii</b>
<b>List of tables .....</b>	<b>ix</b>
<b>1 Introduction .....</b>	<b>1</b>
1.1 Purpose and Scope .....	1
1.2 Recommendations for Product Specification .....	1
1.3 References .....	2
1.3.1 Applicable Documents .....	2
1.3.2 Reference Documents.....	3
1.4 Acronyms .....	3
<b>2 Product format and metadata .....</b>	<b>5</b>
2.1 Data format.....	5
2.2 Filename convention .....	5
2.2.1 CCI Project .....	6
2.2.2 Processing level.....	6
2.2.3 Data Type .....	7
2.2.4 Product String .....	7
2.2.5 Additional Segregator .....	7
2.3 Data access.....	7
2.4 Attributes.....	10
2.4.1 Global attributes .....	10
2.4.2 Variable attributes .....	14
<b>3 Spatial and temporal resolution, grid format and projection .....</b>	<b>23</b>
3.1 Spatial resolution.....	23
3.2 Temporal resolution .....	23
3.3 Grid format, map projection and coverage .....	23
<b>4 Error budget and uncertainties .....</b>	<b>24</b>
4.1 Characterizing error and error budgeting.....	24
4.2 Data format for uncertainty information .....	24
<b>5 Quality indicators and flags.....</b>	<b>25</b>
5.1 Quality indicators .....	25
<b>6 Summary .....</b>	<b>26</b>

## List of figures

No table of figures entries found.



## List of tables

Table 1 - Details of processing level naming conventions taken from [RD02] -----	7
Table 2 - Data access-----	8
Table 3 - List of global attributes. The contents of the first four columns of this table are reproduced from CCI Data Standards Issue 2.0 [RD02]. -----	14
Table 4 - List of variable attributes. The contents of the first three columns of this table are reproduced from CCI Data Standards 2.3 Document [RD02]. -----	15
Table 5 -Summary of the specifications of the last dataset CCI+SSS project (dataset year3). . --	26



## 1 Introduction

### 1.1 Purpose and Scope

---

The purpose of this document is to convert the user requirements, summarized in the User Requirement Document (URD, [AD01]), into a detailed set of Sea Surface Salinity (SSS) product specifications of the Sea Surface Salinity Climate Change Initiative (CCI+SSS) project.

The PSD provides results from a detailed analysis of the requirements of current and future users of satellite SSS. The survey aims to involve users in the development process of the CCI+SSS product and to understand their needs prior to the start of the product development.

The PSD connects the recommendations from the URD with the aim to produce a detailed set of product specifications that respond to the user needs and are continuously assessed against their needs.

### 1.2 Recommendations for Product Specification

---

The survey conducted by the project was very detailed and the requirements are widely spread. Therefore, not all aspects of user requirements are covered by the first phase of CCI+SSS. (which coincides with the third programmatic phase of the whole CCI Program).

The goal is to design products that meet as many requirements as possible taking into account the available options. The recommendations derived here from the user consultation relate to a growing and diverse user community and their needs:

- 1) **make high-resolution data available**, to account for the high diversity of requirements for spatio-temporal resolution of the products. The survey results show that the resolution needs strongly depend on the analyzed phenomena ranging from original spatial sampling to 10° and temporal resolution from weekly (daily sampling) to monthly (15 day sampling).
- 2) **Error specification for L4 SSS product, along with error estimation details**, to account for the need of broad uncertainty specification. The CCI+SSS product will contain the random error, systematic error, standard deviation of the bias, as well as good/bad flags computed from different indicators (Xi2, number of outliers).
- 3) **Compatibility between products (L2, L3, L4, other CCI products)**



**Climate Change Initiative+ (CCI+)  
Phase 1**

**Product Specification  
Document**

Ref.: ESA-CCI-PRGM-EOPS-SW-17-0032

Date: 11/19/2021

Version : v2.3

Page: 2 of 36

## 1.3 References

### 1.3.1 Applicable Documents

ID	DOCUMENT	REFERENCE
<b>AD01</b>	User Reference Document (URD)	SSS_cci_D1.1_URD-v2.0
<b>AD02</b>	Climate Research Data Package (CRDP)	SSS_cci-D4.2-CRDP-v2.0



**Climate Change Initiative+ (CCI+)  
Phase 1**

**Product Specification  
Document**

Ref.: ESA-CCI-PRGM-EOPS-SW-17-0032

Date: 11/19/2021

Version : v2.3

Page: 3 of 36

### 1.3.2 Reference Documents

List here all the document that must be read in the conjunction of this document.

ID	DOCUMENT	REFERENCE
<b>RD01</b>	End-to-End ECV Uncertainty Budget	E3UB
<b>RD02</b>	CCI Data Standards 2.3 (26/07/2021)	CCI-PRGM-EOPS-TN-13-009

### 1.4 Acronyms

AD	Applicable Document
ADP	Algorithm Development Plan
ATBD	Algorithm Theoretical Basis Document
CCI	The ESA Climate Change Initiative (CCI) is formally known as the Global Monitoring for Essential Climate Variables (GMECV) element of the European Earth Watch programme
CCI+	Climate Change Initiative Extension (CCI+), is an extension of the CCI over the period 2017–2024
CMUG	Climate Modelling User Group
DARD	Data Access Requirements Document
DOI	Digital Object Identifier
E3UB	End-to-End ECV Uncertainty Budget
EC	European Commission
ECV	Essential Climate Variable
EO	Earth Observation
EOV	Essential Ocean Variable (of the OOPC)
ESM	Earth System Model
NASA	National Aeronautics and Space Administration
ODP	Open Data Portal
PSD	Product Specification Document
PUG	Product User Guide
PVASR	Product Validation and Algorithm Selection Report
PVIR	Product Validation and Intercomparison Report
PVP	Product Validation Plan
RD	Reference Document
SMAP	Soil Moisture Active Passive [mission of NASA]
SMOS	Soil Moisture and Ocean Salinity [satellite of ESA]
SRD	System Requirements Document
SSD	System Specification Document
SSS	Sea Surface Salinity
SVR	System Verification Report



***Climate Change Initiative+ (CCI+)***  
***Phase 1***

**Product Specification  
Document**

Ref.: ESA-CCI-PRGM-EOPS-SW-17-0032

Date: 11/19/2021

Version : v2.3

Page: 4 of 36

UCR/CECR    Uncertainty Characterisation Report (formerly known as the Comprehensive Error  
Characterisation Report)  
URD         User Requirements Document



## 2 Product format and metadata

### 2.1 Data format

---

Users expressed a clear preference for data in NetCDF format [AD01]. NetCDF has many advantages, since it is a self-describing, machine independent data format used in a number of other projects.

Consequently, the primary format of CCI+SSS dataset is NetCDF. CCI, in general produce data according to the CCI Data Standards Requirements in netCDF-4 classic format using Climate and Forecasting (CF) Metadata convention [RD02].

NetCDF format allows the use of various programming languages and tools to read and analyze the data, for example MATLAB, the preferred language chosen by the users. File format and name convention follow the common CCI conventions.

The SSS ECV user products are stored in netCDF-4 (classic) format. They conform with:

- the CCI Data Standard version 2.3 [DSTD]
- the Climate and Forecasting (CF) convention version 1.8
- Attribute Convention for Data Discovery (ACDD) version 1.3
- Infrastructure for Spatial Information in the European Community (INSPIRE) metadata records

### 2.2 Filename convention

---

A common CCI filename convention has been developed and CCI+SSS follows these.

```
ESACCI-<CCI project>-<processing level>-<data type>-<product string>[-<additional segregator>]-<indicative date>-[<indicative time>]-fv<file version>.nc
```

For example, a SSS product with a timestep of one day and a spatial grid size of 25 km version 3.21 (from final phase 1 CRDP) for the first November 2018, created from merged satellite SSS measurements is named:

```
ESACCI-SEASURFACESALINITY-L4-SSS-  
MERGED_OI_7DAY_RUNNINGMEAN_DAILY_25km-20181101-fv3.21.nc
```

Monthly SSS product with a spatial grid size of 25 km with the centered date at the first November is named:



**Climate Change Initiative+ (CCI+)  
Phase 1**

**Product Specification  
Document**

Ref.: ESA-CCI-PRGM-EOPS-SW-17-0032

Date: 11/19/2021

Version : v2.3

Page: 6 of 36

ESACCI-SEASURFACESALINITY-L4-SSS-  
MERGED\_OI\_Monthly\_CENTRED\_15Day\_25km-20181101-fv3.21.nc

The same product but with the centred date at the 15th November:

ESACCI-SEASURFACESALINITY-L4-SSS-  
MERGED\_OI\_Monthly\_CENTRED\_15Day\_25km-20181115-fv3.21.nc

### 2.2.1 CCI Project

The project identifier is set to SSS.

### 2.2.2 Processing level

During the first phase of the CCI+SSS project a Level 4 (L4) product has been provided, a data product created from the analysis of lower level satellite data from SMOS, Aquarius and SMAP that result in gridded high-quality products.

Level	<Processing level> Code	Description
Level 0	L0	Unprocessed and payload data at full resolution. No CCI recommendations regarding formats or content for data at this processing level
Level 1A	L1A	Reconstructed unprocessed instrument data at full resolution, time referenced and annotated with ancillary information, including radiometric and geometric calibration coefficients and georeferencing parameters, computed and appended, but not applied, to L0 data
Level 1B	L1B	Level 1A data processed to sensor units
Level 1C	L1C	Further processed Level 1B data (e.g. correcting radiances, mapping onto a spatial grid)
Level 2	L2	Retrieved environmental variables at the same resolution and location as the level 1 source
Level 2 Pre-processed	L2P	Geophysical variables derived from Level 1 source data at the same resolution and location as Level 1 data, typically in a



		satellite projection with geographic information. These data are the fundamental basis for higher level CCI products.	
Level 3	L3	L2 variables mapped on a defined grid with reduced ancillary data requirements:	
Level 3	L3U	Uncollated L3U: L2 data granules remapped to a space grid without combining any observations from overlapping orbits.	
Level 3	L3C	Collated L3C: Observations combined from a single instrument into a space-time grid	
Level 3	L3S	Super-collated L3S: Observations combined from multiple instruments into a space-time grid	
Level 4	L4	Data set created from an analysis of lower level data that result in gridded, gap-free products	

*Table 1 - Details of processing level naming conventions taken from [RD02]*

### 2.2.3 Data Type

---

Here, the main data type in the dataset is described, SSS for Sea Surface Salinity.

### 2.2.4 Product String

---

The product string depends on the processing level. During the course of phase 1 L4 is adopted, therefore, the product string is MERGED since 3 satellite data (SMOS, SMAP and AQUARIUS) were considered to generate the products.

### 2.2.5 Additional Segregator

---

The additional segregator describes an optional part of the filename.

## 2.3 Data access

---

Based on the User Requirement Survey [AD01], the user community prefer accessing data using a File Transfer Protocol (FTP) with a dedicated FTP connection. Furthermore, users require data products available at multiple resolutions. During phase 1, two L4 products have been provided with 1) daily time step based on a 7-day running mean and 2) a monthly mean.

The archive of SSS ECV data product is accessible through an FTP server hosted by CEDA using the following parameters:





**Climate Change Initiative+ (CCI+)  
Phase 1**

**Product Specification  
Document**

Ref.: ESA-CCI-PRGM-EOPS-SW-17-0032  
Date: 11/19/2021  
Version : v2.3  
Page: 8 of 36

Parameter	Value
Ftp server name	<a href="ftp://anon-ftp.ceda.ac.uk">ftp://anon-ftp.ceda.ac.uk</a>
Login name	anonymous
<b>Year 1</b>	
Full path	<a href="ftp://anon-ftp.ceda.ac.uk/neodc/esacci/sea_surface_salinity/data/v01.8/">ftp://anon-ftp.ceda.ac.uk/neodc/esacci/sea_surface_salinity/data/v01.8/</a>
DOI	<a href="http://dx.doi.org/10.5285/9ef0ebf847564c2eabe62cac4899ec41">http://dx.doi.org/10.5285/9ef0ebf847564c2eabe62cac4899ec41</a>
<b>Year 2</b>	
Full path	<a href="ftp://anon-ftp.ceda.ac.uk/neodc/esacci/sea_surface_salinity/data/v02.31/">ftp://anon-ftp.ceda.ac.uk/neodc/esacci/sea_surface_salinity/data/v02.31/</a>
DOI	<a href="http://dx.doi.org/10.5285/4ce685bff631459fb2a30faa699f3fc5">http://dx.doi.org/10.5285/4ce685bff631459fb2a30faa699f3fc5</a>
<b>Year 3</b>	
Full path	<a href="ftp://anon-ftp.ceda.ac.uk/neodc/esacci/sea_surface_salinity/data/v03.21/">ftp://anon-ftp.ceda.ac.uk/neodc/esacci/sea_surface_salinity/data/v03.21/</a>
DOI	<a href="http://dx.doi.org/10.5285/5920a2c77e3c45339477acd31ce62c3c">http://dx.doi.org/10.5285/5920a2c77e3c45339477acd31ce62c3c</a>

Table 2 - Data access

The full directory structure is the following (example for Year 1 CRDP):

**Index of /neodc/esacci/sea\_surface\_salinity/data/v01.8/**

[parent directory]

Name	Size	Date Modified
30days/		11/25/19, 2:21:00 PM
7days/		11/25/19, 2:21:00 PM



**Climate Change Initiative+ (CCI+)  
Phase 1**

**Product Specification  
Document**

Ref.: ESA-CCI-PRGM-EOPS-SW-17-0032

Date: 11/19/2021

Version : v2.3

Page: 9 of 36

### Index of /neodc/esacci/sea\_surface\_salinity/data/v01.8/30days/

[parent directory]

	Name	Size	Date Modified
<input type="checkbox"/>	00README_catalogue_and_licence.txt	899 B	11/25/19, 2:21:00 PM
<input type="checkbox"/>	2010/		11/6/19, 5:42:00 PM
<input type="checkbox"/>	2011/		11/6/19, 5:34:00 PM
<input type="checkbox"/>	2012/		11/6/19, 5:38:00 PM
<input type="checkbox"/>	2013/		11/6/19, 5:39:00 PM
<input type="checkbox"/>	2014/		11/6/19, 5:41:00 PM
<input type="checkbox"/>	2015/		11/6/19, 5:37:00 PM
<input type="checkbox"/>	2016/		11/6/19, 5:38:00 PM
<input type="checkbox"/>	2017/		11/6/19, 5:39:00 PM
<input type="checkbox"/>	2018/		11/6/19, 5:40:00 PM

The data can be accessed via a web browser.

Under Linux operating system, the command line 'lftp' can be used:

```
lftp anon
```



## 2.4 Attributes

Attributes are metadata stored in the NetCDF files. Here, a distinction is made between global and variable attributes. The latter are specific for each variable and differ between data- and NetCDF files. On the other hand, global attributes apply to the whole content of the NetCDF file.

### 2.4.1 Global attributes

Name	Data Type	Description	CCI+SSS Definition
title	string	description of the data set	ESA CCI Sea Surface Salinity ECV produced at a spatial resolution of 50 km and time resolution of 1 week and spatially resampled on 25 km EASE grid and 1 day of time sampling
institution	string	Institution where the data was produced	ACRI-ST; LOCEAN
source	string	Original data sources	SMOS CCI v3 L2OS reprocessing (ERA5,ref OTT SSS:ISAS, RFI filtering) from DPGS L1 v620, L2OS v662 modified as in DOI:10.1109/tgrs.2020.3030488, SMAP L2 RSS v4.0 - DOI:10.5067/SMP40-2SOCS, Aquarius L3 v5.0 - DOI:10.5067/AQR50-3SQCS
history	string	processing history of data set	Empty field
references	string	references to ATBD	<a href="http://cci.esa.int/salinity-DOI:10.5285/9ef0ebf847564c2eabe62cac4899ec41">http://cci.esa.int/salinity-DOI:10.5285/9ef0ebf847564c2eabe62cac4899ec41</a>
tracking_id	string	a Universal Unique Identifier value	e.g. c9084d41-f887-45de-91bc-925140bb24a2
Conventions	string	the CF version	CF-1.8
product_version	string	Product version of this data file	n{1,}[.n{1,}], e.g. 01.8



**Climate Change Initiative+ (CCI+)  
Phase 1**

**Product Specification  
Document**

Ref.: ESA-CCI-PRGM-EOPS-SW-17-0032

Date: 11/19/2021

Version : v2.3

Page: 11 of 36

format_version	string		CCI Data Standards v2.3
summary	string	a paragraph describing the data set	ESA CCI Sea Surface Salinity
keywords	string	a comma separated list of keywords and phrases	Ocean; Ocean Salinity; Sea Surface Salinity; Satellite
key_variables	string	key primary variables in the file	sss,sss_random_error
id	string	file name, file identification	e.g. ESACCI-SEASURFACESALINITY-L4-SSS-MERGED_OI_7DAY_RUNNINGMEAN_DAILY_25km-20181101-fv3.21.nc
naming authority	string		European Space Agency - ESA Climate Office
keywords_vocabulary	string		NASA Global Change Master Directory (GCMD) Science Keywords
cdm_data_type	string	The THREDDS data type appropriate for this data set.	Grid
comment	string	Various information about the data set	<p><u>Field used in Year 3 dataset:</u></p> <p>The following caveats must be considered: 1) Products have not been fully optimised at very high latitudes, 2) There is a systematic global underestimation of ~0.1 pss early 2010 that gradually disappears over the year (related to the SMOS mission commissioning phase), 3) Products are in general of better quality after 2015 due to the inclusion of SMAP data and reduced contaminations (RFI, sun) on SMOS data. We (Mngt_CCI-Salinity@argans.co.uk) are very keen to get users feedbacks about these products</p>



**Climate Change Initiative+ (CCI+)  
Phase 1**

**Product Specification  
Document**

Ref.: ESA-CCI-PRGM-EOPS-SW-17-0032

Date: 11/19/2021

Version : v2.3

Page: 12 of 36

platform	string	Satellite names	PROTEUS; SAC-D,SMAP
sensor	string	Sensor names	SMOS/MIRAS; Aquarius; SMAP
date_created	string	the date on which the data was created	yyyymmddThhmmssZ
creation_time	string	the date on which the data was created	dd-mmm-yyyy hh:mm:ss
date_modified	string	the date on which the data was modified	
creator_name	string	Name of the creator	ACRI-ST; LOCEAN
creator_url	string	Contact of the creator	<a href="https://climate.esa.int/fr/projects/sea-surface-salinity/">https://climate.esa.int/fr/projects/sea-surface-salinity/</a>
creator_email	string	Contact of the creator	jean-luc.vergely@acri-st.fr
project	string	the scientific project that produced the data: "Climate Change Initiative – European Space Agency"	Climate Change Initiative - European Space Agency
geospatial_lat_min	float	Decimal degrees North, Range: -90 to 90	-83.5171356201172



**Climate Change Initiative+ (CCI+)  
Phase 1**

**Product Specification  
Document**

Ref.: ESA-CCI-PRGM-EOPS-SW-17-0032

Date: 11/19/2021

Version : v2.3

Page: 13 of 36

geospatial_lat_max	float	Decimal degrees North, Range: -90 to 90	83.5171356201172
geospatial_lon_min	float	Decimal degrees East, Range: -180 to 180	-179.870315551758
geospatial_lon_max	float	Decimal degrees East, Range: -180 to 180	179.870315551758
geospatial_vertical_min	float	Vertical bounding min	0
geospatial_vertical_max	float	Vertical bounding max	0
geospatial_lat_units	string	Unit in latitude	degrees_north
geospatial_lon_units	string	Unit in longitude	degrees_east
time_coverage_start	string	Time of the first measurement in the data file. Time format is ISO 8601.	yyyyMMddThhmmssZ e.g. 20181028T000000Z
time_coverage_end	string	Time of the last measurement in the data file. Time format is ISO 8601.	yyyyMMddThhmmssZ e.g. 20181104T235959Z
time_coverage_duration	string	Length of time coverage	P1M (monthly) P7D (weekly)
time_coverage_resolution	string	Time resolution	P15D (monthly) P1D (weekly)



spatial_resolution	string	Spatial resolution	50km
spatial_grid	string	Resolution of the product spatial grid	25km EASE 2 cylindrical grid
standard_name_vocabulary	string	the name of the controlled vocabulary from which variable standard names are taken	NetCDF Climate and Forecast (CF) Metadata Conventions Version 1.8
licence	string	describe the restrictions to data access and distribution	ESA CCI Data Policy: free and open access

*Table 3 - List of global attributes. The contents of the first four columns of this table are reproduced from CCI Data Standards Issue 2.0 [RD02].*

## 2.4.2 Variable attributes

Both weekly and monthly products have the same list of variables. They are detailed hereafter with the corresponding netCDF attributes.

Name	Data Type	Description	CCI+SSS Definition
standard_name	string	the standard name of the variable following the CF convention	sea_surface_salinity, longitude, latitude....
_FillValue	same as variable data type	a value used to indicate array elements containing no valid data	NaN or a number
units	string	Description of the units (text). Preferable S.I.	psu, degrees_east, degrees_north....



scale_factor	same as variable data type	a factor needed to convert the variable into S.I. units	
add_offset	same as variable data type	offset needed to convert variable into S.I. units	
long_name	string	a free text descriptive variable name	
valid_min	same as variable data type	Minimum valid value for this variable	
valid_max	same as variable data type	Maximum valid value for this variable	
valid_range	same as variable data type	Range of valid values for this variable (if no valid_min/valid_max is provided)	
ancillary_variables	string	A list of variable names associated to this variable	

*Table 4 - List of variable attributes. The contents of the first three columns of this table are reproduced from CCI Data Standards 2.3 Document [RD02].*

Based on these conventions, the file contains:

1. a map of SSS
2. a corresponding map of uncertainties (named random errors)
3. corresponding maps of quality flags (good/bad flags computed from Xi2 and number of outliers), Ice sea and land sea contamination quality check
4. a corresponding map of the number of outliers
5. the number of SSS in the time interval
6. the percentage of SSS\_variability that is expected to be not explained by the products
7. global attributes





**Climate Change Initiative+ (CCI+)  
Phase 1**

**Product Specification  
Document**

Ref.: ESA-CCI-PRGM-EOPS-SW-17-0032

Date: 11/19/2021

Version : v2.3

Page: 16 of 36

The L4 files contain an area conservative lat-lon map (on EASE2 grid), the products at the different time steps (daily, monthly) files share the same names for variables that appear in both products as well as dimensions (latitude, longitude, SSS, QF etc.):

Dimensions:

The EASE 2 global grid at 25 km covers:

584 pixels in the latitude direction (lat)

1388 pixels in the longitude direction (lon)

Variables are also indexed by time with:

1 corresponding to the coverage date (time)

Latitude:

	Value
<b>Variable name</b>	Lat
<b>Dimensions</b>	lat (584)
<b>Data type</b>	float32 (4 bytes)
long_name	latitude
standard_name	latitude
units	degrees_north
valid_min	-90
valid_max	90
_FillValue	NaN

Longitude:

	Value
<b>Variable name</b>	lon



**Climate Change Initiative+ (CCI+)  
Phase 1**

**Product Specification  
Document**

Ref.: ESA-CCI-PRGM-EOPS-SW-17-0032

Date: 11/19/2021

Version : v2.3

Page: 17 of 36

<b>Dimensions</b>	lon (1388)
<b>Data type</b>	float32 (4 bytes)
long_name	longitude
standard_name	longitude
units	degrees_east
valid_min	-180
valid_max	180
_FillValue	NaN



**Climate Change Initiative+ (CCI+)  
Phase 1**

**Product Specification  
Document**

Ref.: ESA-CCI-PRGM-EOPS-SW-17-0032

Date: 11/19/2021

Version : v2.3

Page: 18 of 36

**Time:**

	Value
<b>Variable name</b>	time
<b>Dimensions</b>	time (1)
<b>Data type</b>	float32 (4 bytes)
long_name	time
standard_name	time
units	days since 1970-01-01 00:00:00 UTC
calendar	standard
_FillValue	NaN

**Number of observations:**

	Value
<b>Variable name</b>	total_nobs
<b>Dimensions</b>	time, lat, lon
<b>Data type</b>	short integer (2 bytes)
long_name	Number of SSS in the time interval
valid_min	0
valid_max	1000
_FillValue	-1



**Climate Change Initiative+ (CCI+)  
Phase 1**

**Product Specification  
Document**

Ref.: ESA-CCI-PRGM-EOPS-SW-17-0032

Date: 11/19/2021

Version : v2.3

Page: 19 of 36

**Number of outliers:**

	Value
<b>Variable name</b>	noutliers
<b>Dimensions</b>	time, lat, lon
<b>Data type</b>	short integer (2 bytes)
long_name	Count of the Number of Outliers within this bin cell
valid_min	0
valid_max	1000
_FillValue	-1

**SSS:**

	Value
<b>Variable name</b>	sss
<b>Dimensions</b>	time, lat, lon
<b>Data type</b>	float32 (4 bytes)
long_name	Multi-Satellite Sea Surface Salinity
standard_name	sea_surface_salinity
valid_min	0
valid_max	50
ancillary_variables	noutliers total_nobs sss_qc
_FillValue	NaN



**Climate Change Initiative+ (CCI+)  
Phase 1**

**Product Specification  
Document**

Ref.: ESA-CCI-PRGM-EOPS-SW-17-0032

Date: 11/19/2021

Version : v2.3

Page: 20 of 36

**SSS random error:**

	Value
<b>Variable name</b>	sss_random_error
<b>Dimensions</b>	time, lat, lon
<b>Data type</b>	float32 (4 bytes)
long_name	Sea Surface Salinity Random Error
valid_min	0
valid_max	100
ancillary_variables	pct_var
_FillValue	NaN

**Pct\_var:**

	Value
<b>Variable name</b>	pct_var
<b>Dimensions</b>	time, lat, lon
<b>Data type</b>	float32 (4 bytes)
long_name	Percentage of SSS_variability that is expected to be not explained by the products
valid_min	0
valid_max	100
units	%
_FillValue	NaN



**Climate Change Initiative+ (CCI+)  
Phase 1**

**Product Specification  
Document**

Ref.: ESA-CCI-PRGM-EOPS-SW-17-0032

Date: 11/19/2021

Version : v2.3

Page: 21 of 36

**SSS quality indicator:**

	Value
<b>Variable name</b>	sss_qc
<b>Dimensions</b>	time, lat, lon
<b>Data type</b>	byte
long_name	Sea Surface Salinity Quality, 0=Good; 1=Bad
valid_min	0
valid_max	1

**Land sea contamination quality check:**

	Value
<b>Variable name</b>	lsc_qc
<b>Dimensions</b>	time, lat, lon
<b>Data type</b>	byte
long_name	Land Sea Contamination Quality Check, 0=Good; 1=Bad
valid_min	0
valid_max	1



**Climate Change Initiative+ (CCI+)  
Phase 1**

**Product Specification  
Document**

Ref.: ESA-CCI-PRGM-EOPS-SW-17-0032

Date: 11/19/2021

Version : v2.3

Page: 22 of 36

**Ice sea contamination quality check:**

	Value
<b>Variable name</b>	isc_qc
<b>Dimensions</b>	time, lat, lon
<b>Data type</b>	byte
long_name	Ice Sea Contamination Quality Check, 0=Good; 1=Bad
valid_min	0
valid_max	1



## 3 Spatial and temporal resolution, grid format and projection

The majority of users have spoken out for a high resolution on temporal and spatial scale being able to cope with the most reasonable accuracy possible at this resolution. Here some users wanted high-level data products (L3 and L4) while other users preferred to have low level products (L2).

Within Phase 1, the CCI+SSS project wants to make processed L4 data accessible. Lower-level processed data products based on the different satellites can be accessed via ESA or other websites. Within Phase 2 the CCI+SSS project is planning to provide also debiased L2 and L3 data products.

### 3.1 Spatial resolution

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To analyze at least mesoscale processes, many users require higher spatial resolution (1-100 km) than users who focus on large scale processes (> 100 km). Based on the URD and based on the capabilities of the different L-Band sensors, a specification of interpolated 25 km resolution data based on 75 km resolution seems achievable.

### 3.2 Temporal resolution

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Corresponding to the requirements regarding spatial resolution, the requirements for temporal resolution varied dependent on the research interest. There was no clear majority for the queried resolutions but a tendency to at least weekly data products.

Based on the URD and the capabilities of the sensors (SMOS & SMAP – 3-5 day global coverage, Aquarius 7 days almost global coverage), it seemed sensible to offer a product with daily timesteps with a 7-day window.

For users who require lower temporal resolution a second product is available with a resolution of one month centred 1) at the first of each month and 2) centred at the 15th day of each month. The latter is comparable with climatological means.

### 3.3 Grid format, map projection and coverage

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The majority of users have spoken out for data with a global coverage on a regular latitude-longitude grid. The CCI+SSS product files are delivered on the global (Cylindrical) Equal-Area Scalable Earth Grid 2.0 (EASE 2), since it is used for other satellite SSS products and therefore favors the compatibility between different data products.





## 4 Error budget and uncertainties

In order to characterize errors in the final product, analysis of the various sources of error need to be conducted. Divergent user responses indicate that there is no one way of communicating uncertainties that will suit everyone.

But the majority of users require random noise and systematic errors for each grid point as well as detailed information about the error budget and bias correction.

### 4.1 Characterizing error and error budgeting

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Error characterization and budgeting is described in the End-to-End ECV Uncertainty Budget document (E3UB), but to summarize, the uncertainty can be generally grouped into the following primary categories:

- uncertainties due to the measurement instrument
- systematic errors in the retrieval algorithm
- unknown uncertainties (e.g., spatial-temporal sampling errors)

Errors in each of these sources need to be propagated through the processing pixel by pixel resulting in an error budget for each SSS grid point.

During the first phase of the CCI+SSS project, data sets include information about random errors and number of outliers.. Systematic errors are not available in the final L4 product as it appeared in the previous versions to be very confusing for the users. Error estimation for the L4 CCI+SSS product is described in the End to End ECV Uncertainty Document.

### 4.2 Data format for uncertainty information

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The uncertainty products are stored directly alongside the product in NetCDF, encoding the uncertainty information as additional variable in NetCDF and bin them to their associated variable by attributes and naming convention. This is compatible with the CF conventions.



**Climate Change Initiative+ (CCI+)  
Phase 1**

**Product Specification  
Document**

Ref.: ESA-CCI-PRGM-EOPS-SW-17-0032

Date: 11/19/2021

Version : v2.3

Page: 25 of 36

## 5 Quality indicators and flags

### 5.1 Quality indicators

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Based on the user requirements [AD001], the L4 CCI+SSS product must have quality indicators. Users prefer to have data flagged dependent on their quality. In the case of the L4 product released during the first phase of the CCI+SSS project, three flags are provided, one on the SSS quality, another one on the possible land-sea contamination and a last one on the possible ice-sea contamination. For production, a detailed documentation is needed including all steps in the data and product delivery chain. Furthermore, uncertainty information is essential for the users.



## 6 Summary

The aim of this document was to transform the user requirements summarized in the URD into a set of product specifications for input into Task 2 (algorithm development etc.) of the CCI+SSS project.

1. Three CCI+SSS versions of L4 product on a regular latitude longitude grid have been provided during the phase 1 of the CCI+SSS project (Table 5 -).
2. Data products include uncertainty information (random error) , , number of outliers, number of observations, PCTVAR).
3. Quality indicators are part of the L4 data.
4. At each step of processing, the error has been quantified, propagated through the processing chain and well documented.
5. Updates of the products have been performed at the end of each of the 3 Years of the CCI+SSS Phase-1 project.
6. Data are produced in CF-compliant NetCDF-v4 format
7. The NetCDF data are distributed through an FTP site.

Level	Decorrelation timescales	Spatial Smoothing scale	Temporal timesteps	Spatial grid size	Coverage
L4	weekly	50 km	daily (based on 7-day running means)	25 km	global 01/2010-10/2020
L4	30 days	50 km	centred at each 1st and 15th day of the month	25 km	global 01/2010-10/2020

*Table 5 -Summary of the specifications of the last dataset CCI+SSS project (dataset year3) .*



***Climate Change Initiative+ (CCI+)***  
***Phase 1***

**Product Specification  
Document**

Ref.: ESA-CCI-PRGM-EOPS-SW-17-0032

Date: 11/19/2021

Version : v2.3

Page: 27 of 36

***End of Document***