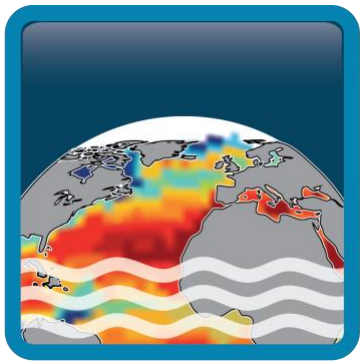
Climate Change Initiative+ (CCI+) Phase 2

Sea Surface Salinity



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Introduction

1.1 Scope of this document

The Climate Change Initiative (CCI) is a program of the European Space Agency aiming to build the longest time series of the Essential Climate Variable (ECV) Sea Surface Salinity (SSS).

This User Requirement Document (URD) aims at reflecting the main requirements of the different user groups. It is an update of the URD written during Phase 1 [AD01] of the project and thus builds up on the knowledge gained during CCI+SSS Phase 1. It fulfils part of the requirements of Task 1 given in the Detailed Proposal [AD02] which specifies that "The Climate Research Group (CRG) will prepare in the early phase of the project an update of the User Requirements Document (URD) for Salinity ECV."
The CMUG review of phase 1 CCI+SSS URD [RD01] brought two considerations that have been taken into account in the redaction of this URD. The first suggestion was to further discuss how survey from phase 1 [AD01] supports requirements expressed by community groups (GCOS, GOOS) and if they show differences, whether they can be interpreted as a change of user requirements. The second suggestion is to discuss which requirements are possible to meet.

1.2 Sea surface salinity observations and users

SSS observations are a key parameter for monitoring the global water cycle (evaporation, precipitation, ice-melting and river runoff). On large scales, surface salinity can be used to infer long-term changes of the global hydrological cycle. Surface salinity, together with surface temperature and air–sea fluxes (heat and momentum) can be used to determine the evolution of the surface expression of fine- to large-scale ocean frontal features and eddies.
Several sensors allow for the observation of SSS from space at global scale: SMOS, Aquarius, SMAP. It is also possible to retrieve salinity in regions with high contrast from AMSR-E. The goal of the European Space Agency (ESA) Climate Change Initiative Sea Surface Salinity (CCI+SSS) project is to optimize satellite SSS time series by merging satellite SSS acquired by various instruments. For the first time, during the CCI+SSS phase 1, SMOS, Aquarius, and SMAP measurements have been combined to produce Level 4 (L4) gridded multi-mission estimates of SSS. Such a combination reduces the noise of satellite SSS fields owing to better sampling and improves the spatial resolution of large mesoscale SSS features (Boutin et al., 2021). The second and current phase commenced in April 2022 and will run for three years. This phase focuses on extending in time and improving the accuracy of the products developed during Phase 1, in exploring further opportunities and limitations in the generation of several multi- sensor data streams.
The target user community can be divided in:
Climate scientists interested in monitoring evolutions of the water cycle,
Ocean and climate modelers who are using SSS to validate or constrain their models,
Physical oceanographers interested in the dynamical functioning of the ocean at regional and global scale and the impact of the upper ocean salinity on others Essential Climate Variable s (ECVs),
Developers of operational applications.

1.3 Structure of the document

This document is structured as follows:
- Chapter 1 Introduction
- Chapter 2 describes the user requirements of organisations, the findings of the Phase 1 user survey, and any feedback from the user community on Phase 1 products
- Chapter 3 provides a summary and discusses the scientific feasibility of meeting the identified user requirements.

1.4 Definitions

We provide below definitions, taken from [RD02], that have been adopted throughout this document:

Measurand: particular quantity subject to measurement. In our case, the salinity, defined as the relative amount of salt dissolved in sea water (corresponding to gram of salt per kilogram of sea water) at the sea surface.

Error: result of a measurement minus a true value of the measurand. Since the 'true' value of the measurand is not known, the 'true' value of the error is unreachable.

Uncertainty: parameter, associated with the result of a measurement, that characterizes the dispersion of the values that could reasonably be attributed to the measurand. Uncertainty of measurement comprises, in general, many components. In the ase of Round Robin (RR) methodology, since measurements are validated by comparisons with measurements in the fields, 'experimental standard deviations' classically evaluated from the statistical distribution of the results of series of measurements realized in the same conditions, cannot be estimated. Hence, in the case of RR, the uncertainty is evaluated from assumed probability distributions of the measurand derived, with some uncertainty, from in situ measurements.

In [RD02], 'it is understood that the result of the measurement is the best estimate of the value of the measurand, and that all components of uncertainty, including those arising from systematic effects, such as components associated with corrections and reference standards, contribute to the dispersion'. In the case of satellite radiometric measurements, the absolute calibration of the SSS is not well known and important differences between the various satellite SSS come from the different systematic corrections that are applied. As a consequence, we will distinguish between 'uncertainties associated with systematic effects' (that can be quantified by a bias) from the 'uncertainties associated with random errors' coming from the noise of the measurements (linked to the radiometric resolution), from errors that are not well characterized given the present knowledge of the sources of errors.

Accuracy : It represent the closeness of the agreement between the result of a measurement and a true value of the measurand. "Accuracy" is a qualitative concept and the term precision should not be used for "accuracy".

Discrepancy: The difference between the data product and the validation value.

Precision: The difference between one result and the mean of several results obtained by the same method, i.e. reproducibility (includes non-systematic errors only).

Satellite SSS: Sea Surface Salinity within the first centimetre of the sea surface, by nature integrated over a horizontal surface that depends on the radiometer characteristics and on the data processing.

In-situ SSS: Near Surface Salinity measured at several cm to several meter depth.

1.5 Salinity unit

According to UNESCO (1985) [RD03], the practical salinity scale, defined as a conductivity ratio, has no units.
The discomfort of handling and describing in publications, reports, or nomenclatures, a physical quantity without a unit, has led to different practices and some confusion about the proper use of salinity. This is probably the reason why the latest GCOS 2022 report [RD05] indicates salinity units as: psu, pss, g/Kg, or no unit.

So we recommend 'no unit' in case it does not bring any confusion and 'pss' when it could be confusing (eg when dealing with a ratio like Kelvins/pss).

To be compliant with the CF metadata conventions (designed to promote the processing and sharing of files created with the NETCDF API), the units in the netCDF files must be compatible with a library called udunits2 which rely on the International System of Units. For salinity, the unit "0.001" must be used.

1.6 References

1.6.1 Applicable Documents

ID	Document	Reference
AD01	User Requirement Document (URD) phase-1	SSS_cci-D1.2-URD-v2r0
AD02	Main detailed proposal CCI+SSS phase 2	ESA_CCI+_CCN_MAIN-DETAILED-PROPOSAL
AD03	Climate Assessment Report (CAR) Customer. Phase 1. v3.2	SSS_cci-D5.1-CAR-v3.2
AD04	Product Specification Document (PSD)	SSS_cci-D1.2-PSD-v2r3

1.6.2 Reference Documents

ID	Document	Reference
RD01	CMUG CCI+Deliverable 1.1: Meeting the needs of the Climate Community – Requirements (v2.2) available at https://climate.esa.int/media/documents/CMUG_Baseline_Requirements_D1.1_v2.2_EUBGoPz.pdf	
RD02	Bureau International des Poids et Mesures, Guide to the Expression of Uncertainty in Measurement (GUM), JCGM 100:2008, 2008. Available online at http://www.bipm.org/en/publications/guides/gum.html	
RD03	The international system of units (SI) in oceanography, UNESCO Technical Papers No. 45, IAPSO Pub. Sci. No. 32, Paris, France.	

ID	Document	Reference
RD04	GCOS-200 The Global Observing System for Climate: Implementation Needs. Available online at https://library.wmo.int/opac/doc_num.php?explnum_id=3417	
RD05	The 2022 GCOS Implementation Plan. GCOS-244. Available online at https:/gcos.wmo.int/en/publications/gcos-implementation-plan2022	
RD06	The 2022 GCOS ECVs Requirements. GCOS-245. Available online at https:/gcos.wmo.int/en/publications/gcos-implementation-plan2022	
RD07	EOV Spec Sheet: Sea Surface Salinity. Availaible online at https://goosocean.org/components/com_oe/oe.php?task=download&id=34510&version=1.0&lang=1&format=1	
RD08	obs4MIPs data specifications (ODS) v2.1 https://esgf-node.llnl.gov/site_media/projects/obs4mips/ODSv2p1.pdf	
RD09	CMEMS requirements for the evolution of the Copernicus Satellite Component", February 2017. Available at https://marine.copernicus.eu/sites/default/files/media/pdf/2020-10/CMEMS-requirements-satellites.pdf	
RD10	GODAE Ocean View refined requirements for SSS products. CLS-SMOS-ENSO-18-0169 Technical Note Available at https://www.godae-oceanview.org/files/download.php?m=documents&f=181203104307-SMOSTN2.pdf	

1.7 Acronyms

CCI+	Climate Change Initiative Extension (CCI+), is an extension of the CCI over the period 2017–2024
CMUG	Climate Modelling User Group
CSWG	Climate Science Working Group
DOI	Digital Object Identifier
ECV	Essential Climate Variable
GOOS	Global Ocean Observing System
GCOS	Global Climate Observing System
IOC	Intergovernmental Oceanographic commission (of UNESCO)
NASA	National Aeronautics and Space Administration
PSD	Product Specification Document
SMAP	Soil Moisture Active Passive [mission of NASA)
SMOS	Soil Moisture and Ocean Salinity [satellite of ESA]
SST	Sea Surface Temperature
SSS	Sea Surface Salinity
URD	User Requirement Document

2 USER REQUIREMENTS

In this section the requirements of the SSS data users are reviewed. These requirements are grouped into those expressed by community groups and by scientists surveyed by the project through a user survey in Phase 1, and as ongoing feedback on our products.

2.1.1 Requirement from Global Climate Observing System (GCOS)

The Global Climate Observing System (GCOS) is intended to be a long-term, user-driven operational system capable of providing information on the climate system. GCOS maintains a list of user requirements. An implementation plan was issued in 2016 [RD04]. The requirements have been revised and summarized in the new GCOS 2022 Implementation Plan (GCOS Climate conference in October 2022) [RD05] and ECVs document [RD06]. For salinity, part of the revision is based on exchanges with the CCI+SSS phase 1 community and URDv1.4 from Sea Surface Salinity Climate Change Initiative Phase 1 [AD01]. The current SSS requirements are as follows:

ECV	Frequency	Horizontal resolution	Requirement measurement uncertainty	Stability per decade
Goal	1-3 days	10km	0.1 (at 50km resolution)	0.01 (for 1000km average)
Threshold	7 days	50-100km	0.2	0.1

Table 1 GCOS in situ sea surface salinity requirements in psu reproduced from GCOS 2022 ECV.

Regarding uncertainty, the recommendation is a goal of 0.1 for 50-km spatial average and monthly mean in low-variability regions (where in-situ validation measurements are not subject to significant sampling errors), a threshold is 0.2 for 100-km spatial average and monthly mean in low variability regions. A stability threshold of 0.1 per decade for 1000-km average in low-variability regions is suggested.

2.1.2 Requirements from GOOS

The GOOS (Global Ocean Observing System) Physics and Climate panel, a program executed by the UNESCO Intergovernmental Oceanographic Commission (IOC), is responsible, among other things, for setting the requirements for Essential Ocean Variables (EOVs) to ensure efficiency of a global ocean observing system.

The GOOS requirements [RD07] they have determined for SSS depend on the spatial and temporal scales of the phenomena and are listed in the following:

Phenomena	Air-Sea Flux (including Ice- Sea Flux)	Coastal Shelf exchange process	Front and Eddies	Riverine
Temporal Scales	daily	daily	weekly	monthly
Spatial Scales	100 km	1 km	10 km	50 km
Magnitudes/range of the signal, thresholds	0.01	0.1	0.1	0.1

Table 2 GOOS requirement settings for sea surface salinity depending on its application at January 2017, reproduced from http://goosocean.org/index.php?option=com_oe&task=viewDocumentRecord&docID=1747

2.1.3 Requirements from CMUG

CMUG has undertaken a review of the requirements for the CCI ECVs through direct interactions with expert users and responses to a questionnaire in order to assist the CCI ECV projects and cross-ECV demonstration projects in focusing on the needs of the Climate Modelling Community, Climate Research Community and other expert users of climate data. For SSS, the requirements taken from the CMUG baseline document v2.2 2021 [RD01] are reproduced below. They are within the range of requirements expressed by GCOS in 2016 [RD04] but they are not in line with the 2022 GCOS requirements [RD06].

It has already been pointed out in the CAR from phase 1 [AD03] that these objectives are not achievable : "CMUG also formulated requirements for SSS data, which are close to the GCOS 2016 requirements. At this stage, these requirements cannot be met with satellite retrieved sea surface salinities. An accuracy of 0.01 is even difficult to meet with in situ salinity data.
In the last year of Phase 1 CCI+SSS plans to bring modelers and Earth observation scientists on one table to put together ideas of how to define the user requirements for SSS to fulfil some of the modeler's requirements, e.g., what exactly is needed for various applications, to identify requirement goals and thresholds and to clarify for what purpose satellite-retrieved salinity data are/ can be used in modelling/assimilation studies."

Parameter	Application	Horizontal Resolution	Observing Cycle	Precision	Accuracy	Stability	Error Type (see Table 3)	Source
Sea surface salinity (Bulk surface salinity, skin surface salinity, near surface salinity at stated depth)	GCOS 2016	1-100 km	Hourly to monthly	0.01 psu	0.01 psu	0.001 psu	See EOV specification sheet at www.goosocean.org/eov	CMUG survey
	Trend monitoring Global/Regional	100km/ 10km	1 week	0.01 psu	0.01 psu	0.001 psu	ERRMERG	CMUG survey
	Decadal forecasting	25km	1 week	0.01 psu	0.01 psu	0.001 psu	SSEOB / ERRMERG	BSC
	Seasonal forecasting	25 km	daily	0.01 psu	0.01 psu	0.001 psu	SSEOB / ERRMERG	BSC
	Global reanalyses	25 km	daily	0.01 psu	0.01 psu	0.001 psu	SSEOB / ERRMERG	BSC
	Regional reanalyses	5 km	daily	0.01 psu	0.01 psu	0.001 psu	SSEOB / ERRMERG	Met Office
	Assimilation	5 km	daily	0.01 psu	0.01 psu	0.001 psu	SSEOB / ERRMERG	BSC

Table 3 CMUG 2021 requirements for satellite derived Sea Surface Salinity observations

2.1.4 Requirement from Obs4Mip

Obs4MIPs (Observations for Model Intercomparisons Project) is an activity to make observational products more accessible for climate model intercomparisons and evaluation. It provides data specifications that are closely aligned with CMIP. There are currently no SSS satellite observations available in this data base. A certain number of attributes should be specified (see obs4MIPs data specifications ODS v2.1 [RD08]), but there are no requirements in terms of resolution or uncertainty.

2.1.5 Requirement from CMEMS

The Copernicus Marine Environment Monitoring Service (CMEMS) provides regular and systematic core reference information on the state of the global ocean and regional seas. The 2020 CMEMS requirements [RD09] for the evolution of the Copernicus components states surface salinity is a very important variable required for CMEMS. They consider that potential impact is high but this requires developments or improvements in satellite technology. So they propose that R&D actions should thus be developed to further advance capabilities in observing sea surface salinity from space. Nevertheless, there are no specific requirements regarding the sea surface salinity ECV.

2.1.6 Requirements expressed by operational centers

Assimilation of SSS satellite observations should help reduce the ocean forecast errors in operational systems and complement the existing observations. Nevertheless, dedicated studies showed that important biases in some regions often degrade the solution and thus still limit the use of SSS data by operational centers.

GODAE OceanView [RD09] proposed in 2018 refined requirements for the use of SSS satellite observations by the operational community for data assimilation and forecasting purposes. These requirements rely on assimilation experiments with two different operational systems from Mercator Ocean and Met Office and inputs from recent assimilation studies from GOV centres.

Three series of values are given (the threshold: the minimum requirement to be met to ensure that data are useful; the breakthrough: an intermediate level which, if achieved, would result in a significant improvement for the targeted application; the goal: an ideal requirement above which further improvements are not necessary)

SSS	Horizontal resolution	Temporal resolution	Uncertainty in PSS
threshold	100 km	weekly *(monthly)*	0.2
the breakthrough	50 km	Daily *(weekly)*	0.2
the goal	10 km	daily	0.1

Table 4: Requirements for GOV system taken from the "GODAE Ocean View refined requirements for SSS products; CLS-SMOS-ENSO-18-0169, 2018"

Moreover it is recommended that products should be:

- based on cross calibrated data between ascending and descending passes to minimize again bias,
- available within a day for real time data assimilation as 1-day assimilation window are already implemented in some operational system and will become more common,
- provided with an uncertainty estimation that is as important as the observation value itself for data assimilation applications.

2.1.7 Requirements from survey during CCC+SSS Phase 1

In addition to the requirements listed above, as part of Phase 1 of CCI_SSS the requirements of the community working on SSS or using SSS data were surveyed by means of a questionnaire [AD01]. The questionnaire was designed to poll for information of the participants in terms of research interest and occupation, synergies with other ECVs, and data specifications (resolution, coverage, uncertainty, format, update frequency, etc…). 54 responses were analyzed.

The overall conclusion was that users are aware of current limitations of satellite SSS data and that improved resolutions, error estimates, uncertainty, documentation, and easy access are desired. Detailed conclusions are as follows:

The survey revealed that the majority of users require global spatial coverage and a temporal coverage of at least 9 years.

The resolution requirements vary according to the studied phenomena. About 33% of respondents want data with a temporal resolution of 1-3 days, while for 35% of the respondents weekly data and for 28% monthly data are sufficient.

In terms of spatial resolution, 39% of the respondents want data with 0.25° horizontal resolution, whereas for 28% of them data on a 1°-grid is sufficient.

The uncertainty, and global mean uncertainty between 0.1 and 0.3 was satisfactory.

A preference for NETCDF and FTP access was expressed.

There was no clear preference for the desired level of processing, reflecting the use of the data for different objectives (e.g., L2/L3 prefered for assimilation studies). In terms of update frequency, 6month/1year was the preferred choice, and participants asked for e-mail information as the main way for communicating new updates.

3 User requirements summary and feasibility

Prior to updating the Product Specifications, the feasibility of being able to meet the User Requirements must be discussed. Thus, the following subsections highlight and revise some user requirements.

3.1.1 Measurement uncertainties.

The GCOS implementation plan from 2016 [RD04] stated a target uncertainty of 0.01 for SSS ECV. In their status report they considered that "The requirement for target of 0.1 on 100 km, monthly scales is marginally met by in situ based gridded products (with root-mean-square differences of different in situ based gridded SSS products being close to 0.1 when averaged spatially)…. Some satellite products meet the accuracy requirement as well."

At that time, it was not clear whether GCOS has changed its requirement from 0.01 to 0.1 or whether this is an error in the status report or in the implementation plan.

The GCOS salinity required have been updated in the last GCOS 2022 ECVs requirement document, with an uncertainty goal at 0.1 for 50-km spatial average and monthly mean in low variability regions and an uncertainty threshold of 0.2 for 100-km spatial average and monthly mean in low variability regions. The GCOS requirements appear now much in line with the needs of the research and operational communities, compared to ~~GCOS implementation plan from 2016 [RD04]~~.

The CMUG requirements, taken from the Climate Community Requirements V2.2 report from 2021, state an accuracy of 0.01. Interestingly such a demanding constraint is not necessarily required by the "SSS" community, as expressed by the participants to the user survey: while the target SSS uncertainty expressed by GCOS is 0.1, global mean uncertainty between 0.1 and 0.3 was considered as satisfactory by the users. Moreover, the users would in general prefer a product with high resolution (weekly, 0.25°) and accept higher uncertainty (0.3). This conclusion must be nuanced for the operational centers for which reduced uncertainty is a priority over horizontal resolution. During Phase 2 of the CCI-SSS, discussions with CMUG should ensure that future definition of CMUG needs is meaningful.

3.1.2 Spatial resolution

One conclusion of the user survey in terms of spatial resolution was that it strongly depends on the applications. In terms of spatial resolution, 39% of respondents to the user survey would require a 0.25° horizontal resolution while for 28% of them, data on a 1°-grid is sufficient. We anticipate that resolution requirements or interests could have increased or shifted toward the 0.25° horizontal resolution since 2018, in particular because of the increased resolution of global climate models and operational models.

3.1.3 Quality information

Uncertainty information for each SSS grid points should be characterized fully, including random noise and systematic errors and uncertainties of applied adjustments. In the survey, information about bias correction was most commonly required by respondents. 50% of respondents want to have flags for each/selected quality control checks, which is not possible for datasets at L3 or L4, which are already binned. data assimilation applications, uncertainty estimation is considered as important as the observation value itself. It is worth noting that Information about systematic errors has been removed from the products because it appeared very confusing for the users.

3.1.4 Level of processing

The most common requirement expressed by users is for L4 data (43%), directly followed by requirements for L3 (37%). Some potential users, mainly operational centers, require L2.

3.1.5 Release frequency

Releases every 6 or 12 months seem adequate for most research / validation applications but operational applications require level 2-3 data with quick release of data in near-real time.

3.1.6 Improving polar observations

Finally, the importance of improving resolution and uncertainty in the polar regions is widely emphasized in the GCOS 2022 Implementation plan [RD05]. This is motivated by the need to better understand and monitor the water cycle, fresh water inputs, and impacts on biogeochemistry.

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