



## Product Quality Assurance Document (PQAD)

Global L4 Sea and Sea Ice Surface Temperature  
Climate Data Record, Version 1.0

WP1-PDDP-SST/IST-v1.0

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### History of document modifications

Version	Date	Description of modification	Chapters / Sections
1.0	30/11/2023	First version	All
1.1	13/06/2024	Document amended in response to independent review	All
1.2	25/06/2024	Document refined, proofread, and finalised for publication	All

### List of datasets covered by this document

Deliverable ID	Product title	Product type (CDR, ICDR)	Version number	Delivery date
WP2-FDDP-SST-v1.0	SST/IST CDR L4	CDR	1.0	



## Related documents

Reference ID	Document
D1	Karagali, I. <i>et al.</i> (2024). Global L4 Sea and Sea Ice Surface Temperature Climate Data Records, Version 1.0: Product Quality Assessment Report. Copernicus Climate Change Service. Document ref. C3S2-312b_WP2-FDDP-SST/IST_2024_PQAR_v1.X.
D2	Karagali, I. <i>et al.</i> (2024). Global L4 Sea and Sea Ice Surface Temperature Climate Data Records, Version 1.0: Product User Guide and Specification. Copernicus Climate Change Service. Document ref. C3S2-312b_WP2-FDDP-SST/IST_2024_PUGS_v1.X.
D3	Karagali, I. <i>et al.</i> (2024). Global L4 Sea and Sea Ice Surface Temperature Climate Data Records, Version 1.0: Algorithm Theoretical Basis Document. Copernicus Climate Change Service. Document ref. C3S2-312b_WP2-FDDP-SST/IST_2024_ATBD_v1.X.
D4	Karagali, I. <i>et al.</i> (2024). Global Sea and Ice Surface Temperature ECV: Target Requirements and Gap Analysis Document. Copernicus Climate Change Service. Document ref. C3S2-312b_WP3-TRGAD-SST/IST_2024_TRGAD_v1.X.
D5	Corlett, G. <i>et al.</i> (2014). ESA CCI Phase 1 SST Product Validation Plan. ESA Climate Change Initiative. Document ref. SST_CCI-PVP-UoL-001, <a href="https://climate.esa.int/media/documents/SST_CCI-PVP-UoL-001-Issue_2-signed-accepted.pdf">https://climate.esa.int/media/documents/SST_CCI-PVP-UoL-001-Issue_2-signed-accepted.pdf</a>
D6	Embury, O. <i>et al.</i> (2024). ESA CCI Phase 2 SST Product Validation and Intercomparison Report (PVIR) SST_CCI_D4.1_PVIR_v2.1. Document ref. SST_CCI_D4.1_PVIR_v2.1, <a href="https://climate.esa.int/media/documents/SST_CCI_D4.1_PVIR_v2.1-signed.pdf">https://climate.esa.int/media/documents/SST_CCI_D4.1_PVIR_v2.1-signed.pdf</a>



## Acronyms

Acronym	Definition
AASTI	Arctic and Antarctic Ice Surface Temperatures from AVHRR
ATLAS	Autonomous Temperature Line Acquisition System
ATSR	Along-Track Scanning Radiometer
AVHRR	Advanced Very-High Resolution Radiometer
C3S	Copernicus Climate Change Service
CCI	Climate Change Initiative
CDR	Climate Data Record
CMEMS	Copernicus Marine Service (formerly called the Copernicus Marine Environment Monitoring Service) ( <a href="http://marine.copernicus.eu">http://marine.copernicus.eu</a> )
CRREL	Cold Regions Research Engineering Laboratory
ESA	European Space Agency
GHR SST	Group for High Resolution SST
GMPE	GHR SST Multi-Product Ensemble
GT MBA	Global Tropical Moored Buoy Array
Had IOD	Met Office Hadley Centre Integrated Ocean Database
Had SST	Met Office Hadley Centre Sea Ice and SST
ICDR	Interim Climate Data Record
IC OADS	International Comprehensive Ocean-Atmosphere Dataset ( <a href="http://icoads.noaa.gov/">http://icoads.noaa.gov/</a> )
MD	Matchup Dataset
MMS	Multi-sensor Matchup System
NWP	Numerical Weather Prediction
PIRATA	Prediction and Research Moored Array
RAMA	Research Moored Array for African-Asian-Australian Monsoon Analysis and Prediction
RSD	Robust Standard Deviation
SIMB3	Seasonal Ice Mass Balance Buoy 3
SLSTR	Sea and Land Surface Temperature Radiometer
SST	Sea Surface Temperature
TAO	Tropical Atmosphere Ocean



## General definitions

**CDR** - Climate Data Record, defines a time series of measurements of sufficient length, consistency, and continuity to determine climate variability and change. Further satellite-based CDRs can be segmented into Fundamental CDRs (FCDRs), which are calibrated and quality-controlled sensor data that have been improved over time, and Thematic CDRs (TCDRs), which are geophysical variables derived from the FCDRs, such as sea surface temperature and cloud fraction.

**ICDR** - Interim Climate Data Record, defines a dataset that has been forward processed, using the baselined Climate Data Record algorithm and processing environment but whose consistency and continuity have not been verified. Eventually, it will be necessary to perform a new reprocessing of the CDR and ICDR parts together to guarantee consistency, and the new reprocessed data record will replace the old CDR.

**SIC** - Sea-ice concentration as fraction (percentage) of the sea surface area of the grid cell containing sea-ice.

**SST** - Sea Surface Temperature

**SST<sub>20cm</sub>** - Sea Surface Temperature adjusted for the standard depth of 0.2 m and time representative of the daily mean, representative of the water temperature free, or almost free of any diurnal warming.

**IST** - Sea Ice Surface Temperature, representative of the surface skin of the sea ice.

**Open ocean** - Corresponds to ice-free ocean or containing very little ice (<15 %), thus the surface temperature is classified as sea surface temperature (SST).

**Sea Ice** - Corresponds to ocean surface covered by sea ice (>70%) thus the surface temperature is classified as sea-ice surface temperature (IST).

**MIZ** - Marginal Ice Zone, a part of the seasonal ice zone that varies in width (100 to 200 kilometers) that extends from the ice edge into the ice pack, where waves and swells affect the ice; often characterized by highly variable ice conditions; in general, it is wider in the Antarctic than the Arctic.

**L2P** - Geophysical variables derived from Level 1 source data on the Level 1 grid (typically the satellite swath projection). Ancillary data and metadata added following GHRST Data Specification.

**L3U** - L2 data granules remapped to a regular latitude/longitude grid without combining observations from multiple source files. L3U files will typically be "sparse", corresponding to a single satellite orbit.



**L3C** – SST observations from a single instrument combined into a space-time grid. In this project, a typical L3C file may contain all the observations from a single instrument in a 24-hour period.

**L3S** – SST observations from many instruments combined into a space-time grid. In this project, a typical L3S file may contain all the observations from all available instruments in a 24-hour period.

**L4** – SST observations from multiple instruments using an analysis system (e.g. optimal interpolation) to produce a gridded, gap-free product.



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## Scope of the document

This Product Quality Assurance Document (PQAD) provides a description of the expected whole product validation methodology for the L4 SST/IST Climate Data Record (CDR) and Interim CDR (ICDR), version 1.0, produced by DMI using data from the Along Track Scanning Radiometer (ATSR), advanced Very-High Resolution Radiometer (AVHRR), and Sea Land Surface Temperature Radiometer (SLSTR) from the ESA CCI and C3S projects for the SST component and from the Arctic and Antarctic ice Surface Temperatures from thermal Infrared satellite climate data record version 2.1 (AASTI v2.1) and C3S ICDR for the IST component

Note that this document contains information on the systems, methods and metrics used to test and evaluate the quality of the CDR and ICDR, both during and after production.

## Executive summary

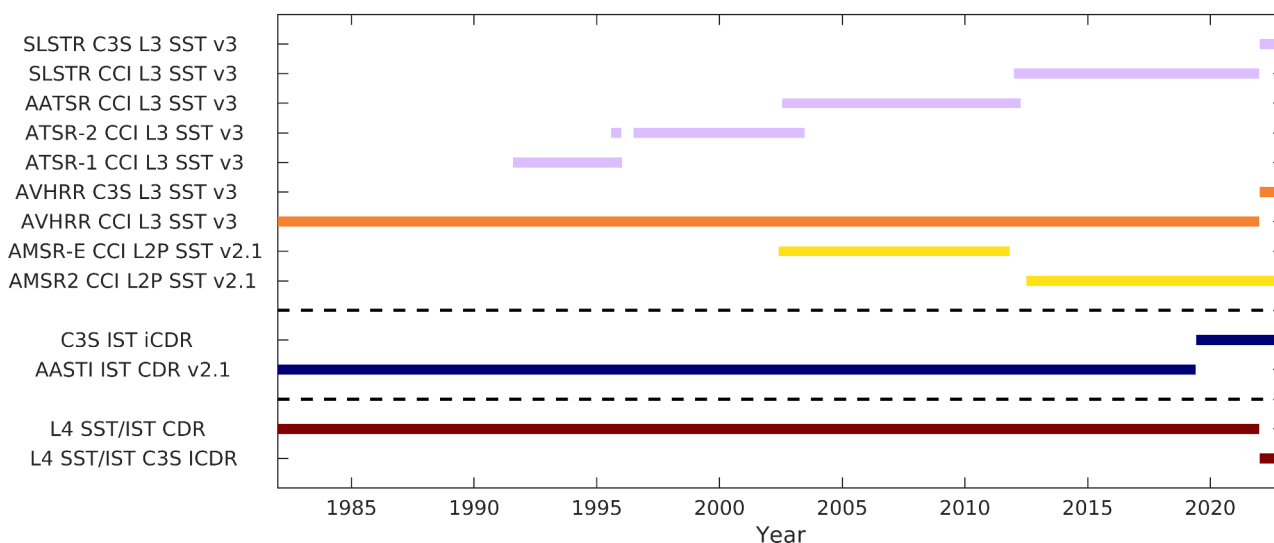
This Product Quality Assurance Document (PQAD) describes the proposed validation and quality assessment methodology for the L4 SST/IST CDR. It gives a brief overview of the validated product (Section 1) followed by a description of the validating datasets (Section 2) and the proposed methodologies (Section 3). Overall, the L4 SST and IST components and their uncertainties will be assessed using a number of different in situ reference datasets (e.g. drifting buoys, moored buoys and Argo floats for the SST component and ice mass balance buoys, drifting ice stations and flight campaigns for the IST component). A multi-sensor matchup system (MMS) will be used to compile the reference measurements and the corresponding SST/IST from the analyses. Robust statistics (median and robust standard deviation) are to be used when assessing differences between the reference data and the L4 SST/IST. Regarding the accuracy and stability for climate assessment, these are defined with respect to reference sensors (drifting buoys for the SST component and ice mass balance buoys and drifting ice stations for the IST component).



## 1. Validated products

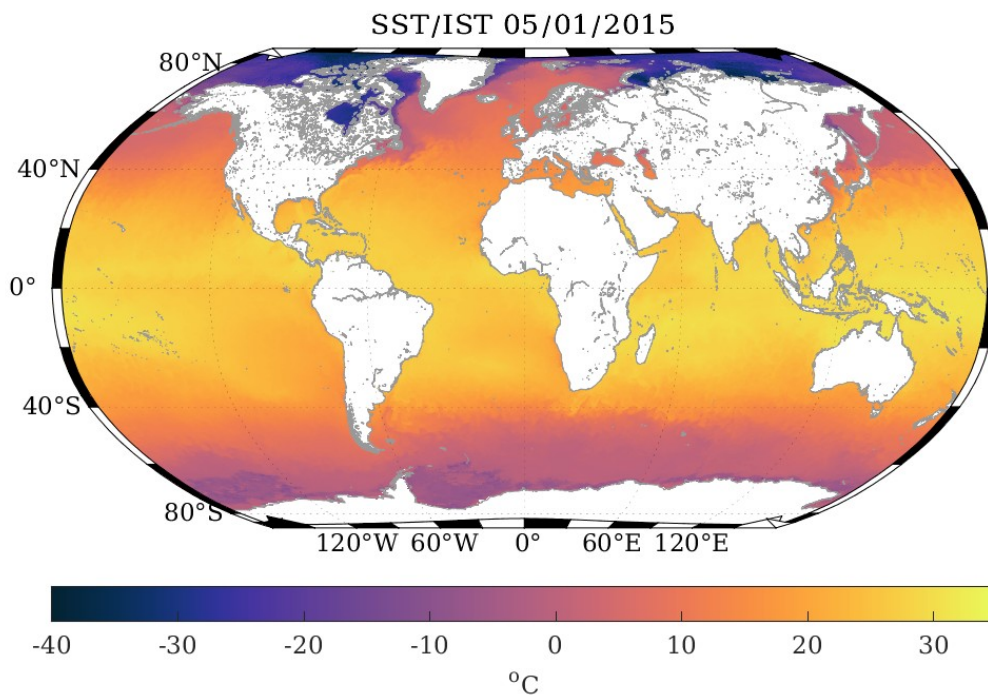
This Quality Assessment Document applies to the version 1.0 daily Global Sea Surface Temperature (SST) and Sea Ice Surface Temperature (IST) Climate Data Record (CDR) and Interim CDR (ICDR) products available at 0.05 degrees spatial resolution. The SST component is representative of the temperature at 20 cm depth while the IST component is representative of the skin temperature. Both ICDR and CDR datasets are generated using the same software and algorithms originally developed within the MyOcean project. These have been improved and adjusted to account for the complex transition from the open ocean SST to the mix between SST and IST in the Marginal Ice Zone (MIZ), and finally to fully sea ice covered regions where only IST is representative. The v1.0 CDR provides a baseline record from the 1982 to end of 2022.

The v1.0 ICDR is produced by C3S as an ongoing extension of the record from Jan 2023 onwards. Together the CCI CDR and C3S ICDR form a continuous dataset as shown in Figure 1 below, the entire timeline of which will undergo validation.



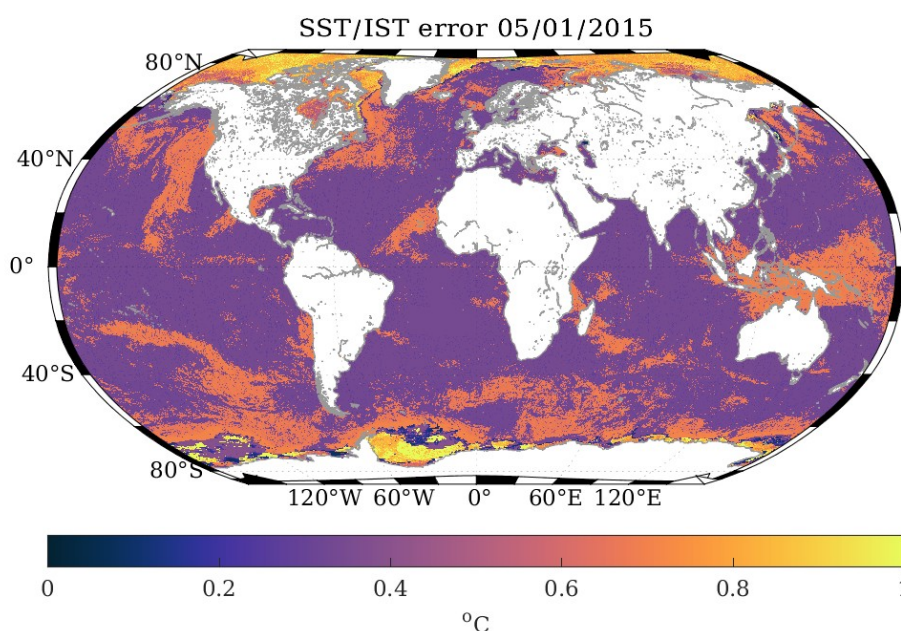
**Figure 1.** Input SST and IST data availability (purple, orange, yellow and blue) from different mission instruments, and CDR /ICDR (dark red) datasets temporal coverage and availability. Mission instrument datasets and C3S product lines are listed on the left hand side. The ICDR provides an extension of the CDR from January 2022 onwards.

An example of the daily global SST/IST field to be validated is shown in Figure 2.



**Figure 2.** Example of one daily global SST/IST field for January 5<sup>th</sup> 2015. Large negative values represent the skin surface temperature over sea-ice. The colour bar indicates surface temperature in degrees C.

Each daily L4 SST/IST is accompanied with an uncertainty estimate, which is a direct output of the OI method. An example of such a field is shown in Figure 3. The standard approach to validate the estimated uncertainties of the L4 SST/IST is to compare them against drifters, where the actual L4 SST minus drifter SST differences are plotted as a function of the OI derived uncertainty estimates.



**Figure 3.** Example of one daily global SST/IST analysis error field for January 1<sup>st</sup> 2015.



## 2. Description of validating datasets

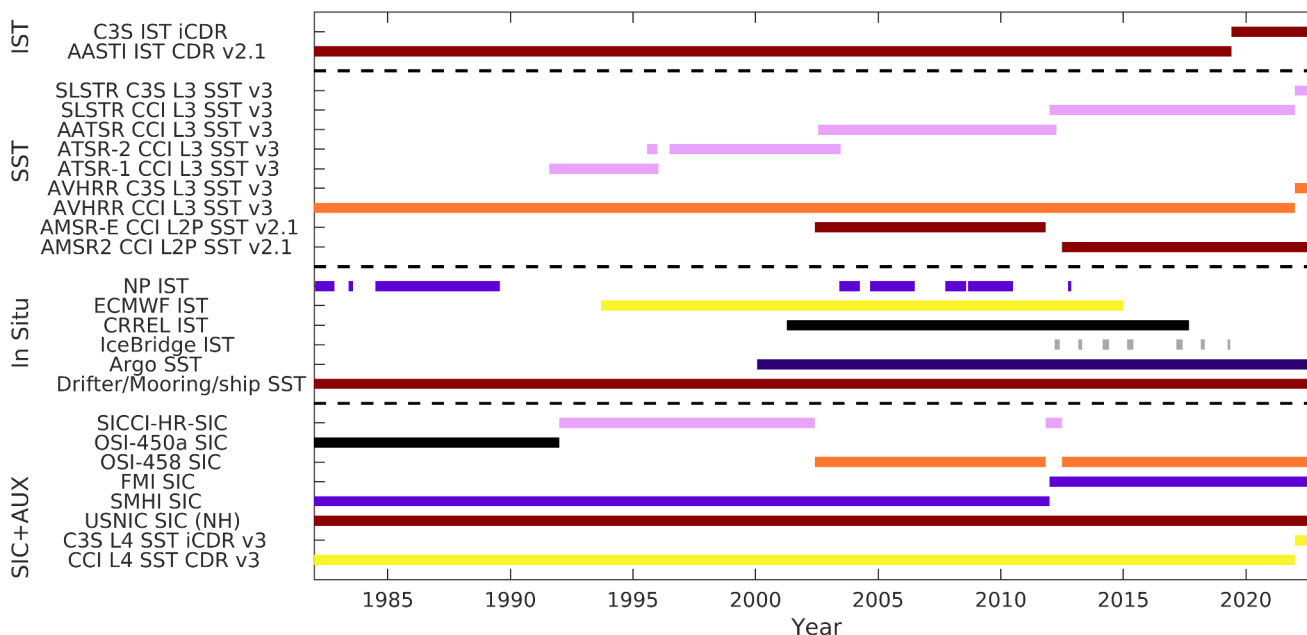
The SST reference dataset used to validate the CDR and ICDR SST component is comprised of in situ SST observations extracted from the Met Office Hadley Centre Integrated Ocean Dataset (HadIOD) v1.2.0.0 (Atkinson et al. 2014). Data are included for the following platform types:

- Drifting buoys (described in Section 2.1),
- Global Tropical Moored Buoy Array (GTMBA, described in Section 2.2),
- Voluntary observing ships (described in Section 2.3),
- Argo floats (described in Section 2.4).

To validate the IST component of the CDR and ICDR, due to lack of in situ measurements of the ice surface temperature, a series of buoys and drifting stations were utilised, typically recording 2 meter air temperatures. Data have been acquired by:

- ECMWF distributed drifting ice buoys (1993–2015, described in Section 2.5.1),
- US Army Cold Regions Research Engineering Laboratory (CRREL) mass balance buoys (2001–2017, described in Section 2.5.2),
- Russian North Pole (NP) drifting ice stations (1982–1989, 2003–2012, described in Section 2.5.3),
- Cryosphere Innovation Seasonal Ice Mass Balance Buoy 3 (SIMB3, described in Section 2.5.3),
- NASA IceBridge Flights. These actually include measurements from an on-board infra-red radiometer and thus are skin surface temperature measurements, and are described in Section 2.6.

The various data types have a range of characteristics with different instrument types, measurement uncertainties, sampling frequency, spatial location, and length of record which are discussed in the following sections. In the present report, the primary in situ types used for SST validation are drifter and GTMBA. Figure 4 shows the temporal extent of the in situ datasets, along with that of the input and auxiliary datasets used for the generation of the SST/IST CDR and iCDR.

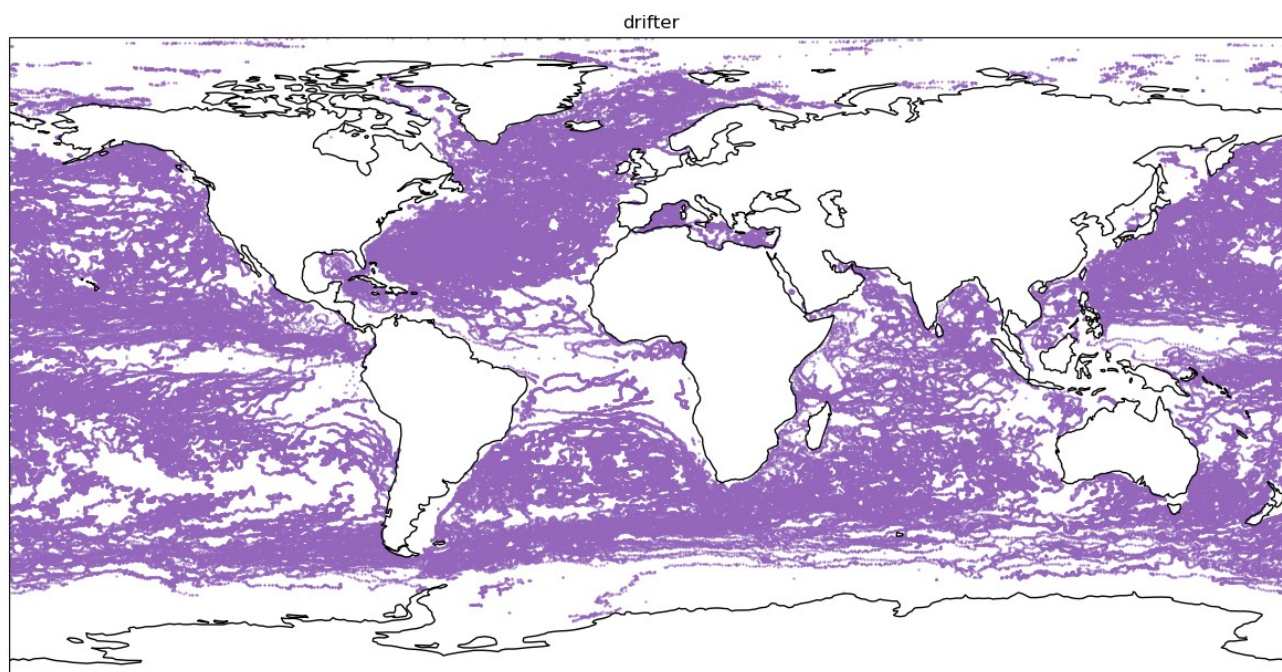


**Figure 4.** Overview of “SST, IST”, and auxiliary input data (for Sea Ice Concentration, “SIC+AUX”) used to generate the L4 SST/IST product, along with the “In Situ” data used for validation.

## 2.1 Drifting buoys

Sub-surface sea temperature measurements are acquired using drifting buoys (or drifters) which provide the most complete – although not uniform - in situ coverage of the world’s oceans. Drifting buoys are surface floats, approximately 30cm in diameter, tethered to sub-surface sea-anchors (or drogues). The drogues ensure the drifters will follow ocean currents (Lumpkin and Pazos, 2007), as if the drogue is lost, the drifter movement will also be affected by wind and waves. These mobile measurement platforms, follow ocean currents, noting that they tend to gather in ocean convergence zones.

All drifters are equipped with an SST sensor located approximately 20 cm below the ocean surface, as well as equipment to transmit collected data to shore via satellite. The standardization of drifting buoy design began in 1982 as part of the World Climate Research Program. The first modern Surface Velocity Program (SVP) drifters were deployed in 1993 and the global drifter program array grew rapidly through the 1990s through to completion in September 2005. The full array provides observations in each 5 x 5 degree grid of open ocean, as shown in Figure 5. For more information on the drifting buoys and an analysis of their accuracy and stability see [D5, D6].



**Figure 5.** Example of drifting buoys used for the validation, for test year 2015. Tracks of the drifting buoys through the global oceans are shown in purple.

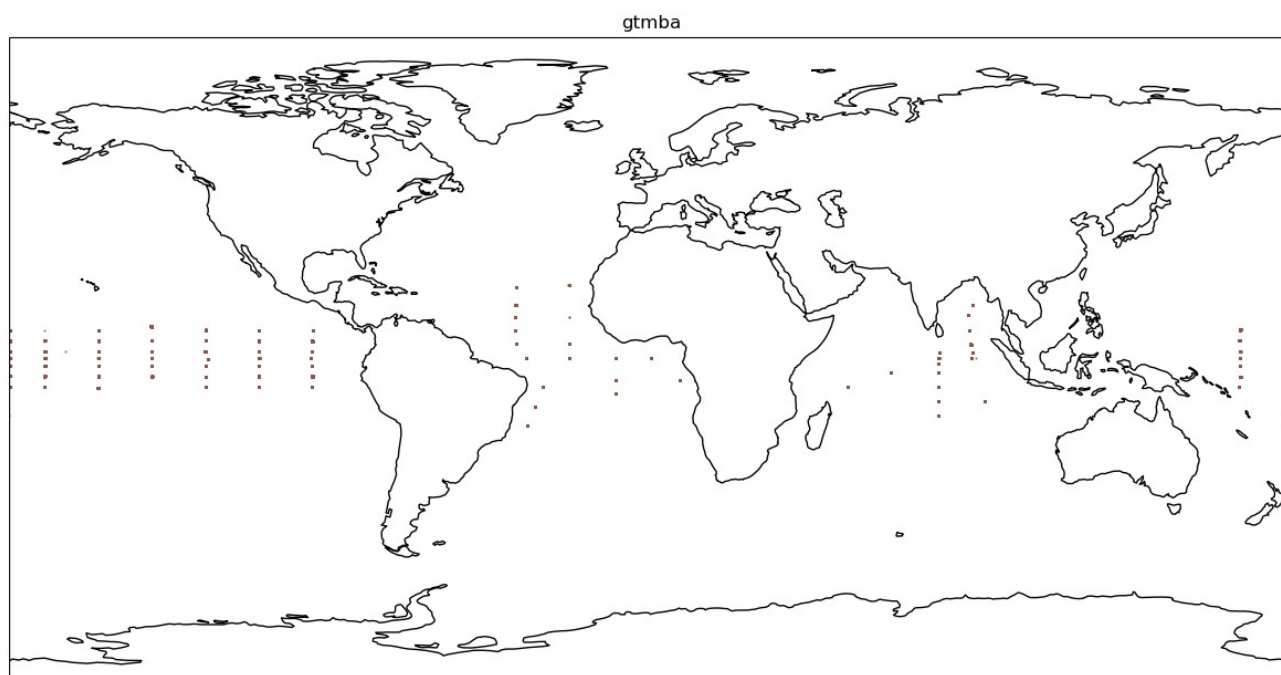
## 2.2 Global Tropical Moored Buoy Array (GTMBA)

In-situ measurements of sea temperature at a depth of 1 m will be used as part of the SST validation activity. These are available from a network of tropical buoys that are managed by three different programmes:

- the Tropical Atmosphere Ocean array in the Pacific ocean (TAO)<sup>1</sup>,
- the Prediction and Research Moored Array (PIRATA) in the Atlantic (Bourlès et al., 2019),
- the Research Moored Array for African-Asian-Australian Monsoon Analysis and Prediction (RAMA) in the Indian Ocean (McPhaden et al. (2009)).

All three networks use Autonomous Temperature Line Acquisition System (ATLAS) moorings which measure a wide range of meteorological and sub-surface parameters, including SST at a depth of 1 m with a resolution of 0.001 K and accuracy of 0.02 K recorded every 10 minutes. Both daily and hourly averages are transmitted while a communication satellite is overhead. This means that hourly measurements are not transmitted for all 24 hours in the day. Full resolution data are stored on the buoys and recovered during service windows. The locations of the arrays are shown in Figure 6. For more information on the moored buoys and an analysis of their accuracy and stability see [D5, D6].

<sup>1</sup> Access to the TAO array information, at [https://tao.ndbc.noaa.gov/proj\\_overview/proj\\_overview\\_ndbc.shtml](https://tao.ndbc.noaa.gov/proj_overview/proj_overview_ndbc.shtml) [last accessed January 9th, 2024].



**Figure 6.** Locations of all moorings in the Tropical Moored Buoy Array.

### 2.3 Voluntary Observing Ships

The Voluntary Observing Ship (VOS) Scheme is an international programme with a membership comprised of WMO member states that recruit ships to take, record and transmit weather observations, including sea surface temperature, whilst at sea. The repository for VOS data (the extent of which is visualised in Figure 7) is the International Comprehensive Ocean-Atmosphere Data Set (ICOADS). Measurements of SST from VOS are available from circa 1850 and onwards. A peak in total VOS was reached in 1984/85 when about 7700 ships worldwide were on the WMO VOS Fleet List. Since then, there has been an irregular but marked decline and in June 1994, the Fleet strength had dropped to about 7200 ships. These numbers have continued to decline and are currently estimated at only about 4000 ships worldwide<sup>2</sup>.

Historically, SST measurements have been made using a combination of methods: using a bucket to haul a sample of water on board in order to take a temperature reading; noting the temperature of water as it comes into the engine room to cool the ships' engines, and via a dedicated hull contact sensor. Measurements are therefore made at various depths while ship's observations are made at the standard synoptic hours of 0000, 0600, 1200 and 1800 UTC and have been for the last several decades.

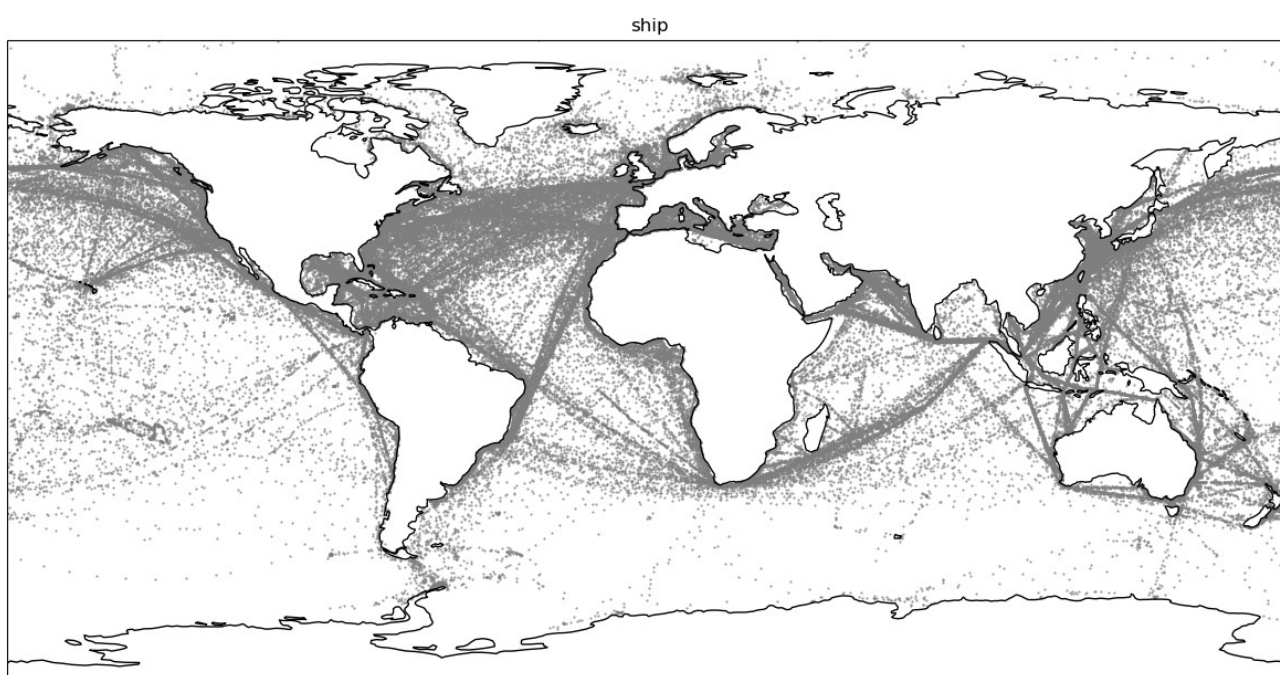
Each ship could be identified using its call sign; where present, call sign information is recorded in ICOADS metadata. However, for many historical reports, this information is absent. Updates to ICOADS v2.0 were taken from the NCEP GTS stream. Call sign information was also recorded in GTS reports until November 2007.

<sup>2</sup> For more information on the VOS scheme, see [http://www.vos.noaa.gov/vos\\_scheme.shtml](http://www.vos.noaa.gov/vos_scheme.shtml) [last accessed 22<sup>nd</sup> April, 2024].



VOSclim<sup>3</sup> is an initiative based on a sub-class of the VOS fleet. VOSclim aims to provide a high-quality subset of marine meteorological data, with extensive associated metadata, to support global climate studies. This sub-class was designed and equipped to provide ground truth data for calibrating satellite observations, and to provide a high quality reference data set for possible re-calibration of observations from the entire VOS fleet. VOSclim first went operational in 2001. The list of participating ships, along with their dates of recruitment and withdrawal (where applicable) from the project is available from the VOSclim ship info webpage<sup>4</sup>.

For more information on the ships and an analysis of their accuracy and stability see [D5, D6].



**Figure 7.** Geographical distribution of observations (grey dots) from ships used for the validation.

## 2.4 Argo floats

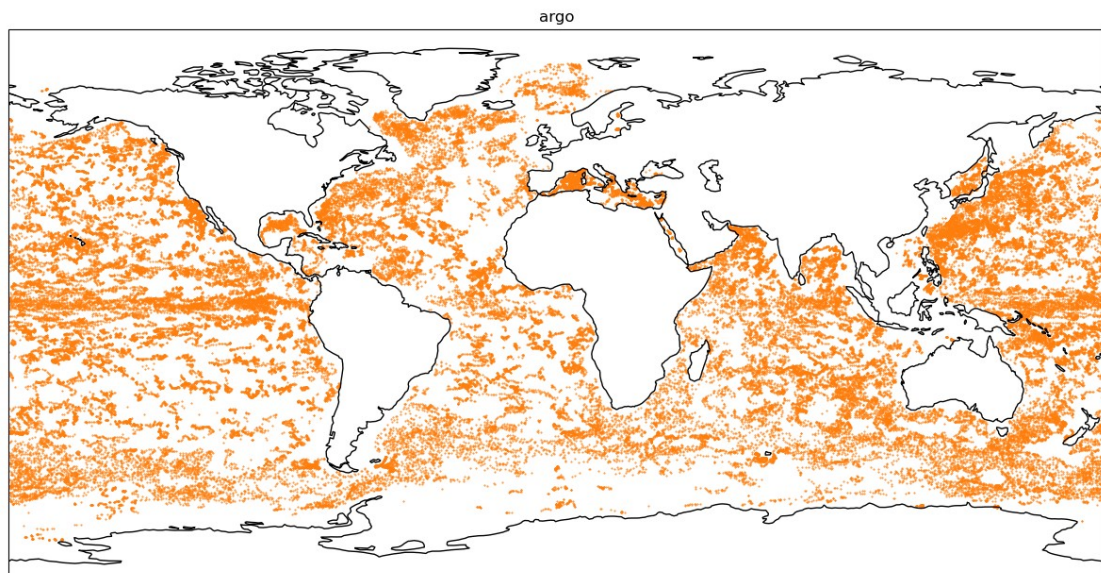
In 1999, the international Argo program was initiated to collect temperature and salinity measurements inside the global ocean using free drifting profiling floats (Roemmich et al., 2009). The Argo floats (Figures 8 and 9) are distributed over the global ice-free ocean and drift with the oceans current and move up and down (usually from the surface to a depth of about 2,000 m). The uppermost temperature measurement is typically measured at a depth of around 5 m and the accuracy of the temperature measurements is very high with uncertainties of 0.002C (Abraham et al., 2013; Kennedy et al., 2014). For validation of the SST component of the combined SST/IST CDR, measurements from the upper 5 m are used. For more information on the Argo buoy measurements and an analysis of their accuracy and stability see [D5, D6].

<sup>3</sup> For more detailed information on VOSclim, see <http://lwf.ncdc.noaa.gov/oa/climate/vosclim/about.html> [last accessed 22<sup>nd</sup> April, 2024].

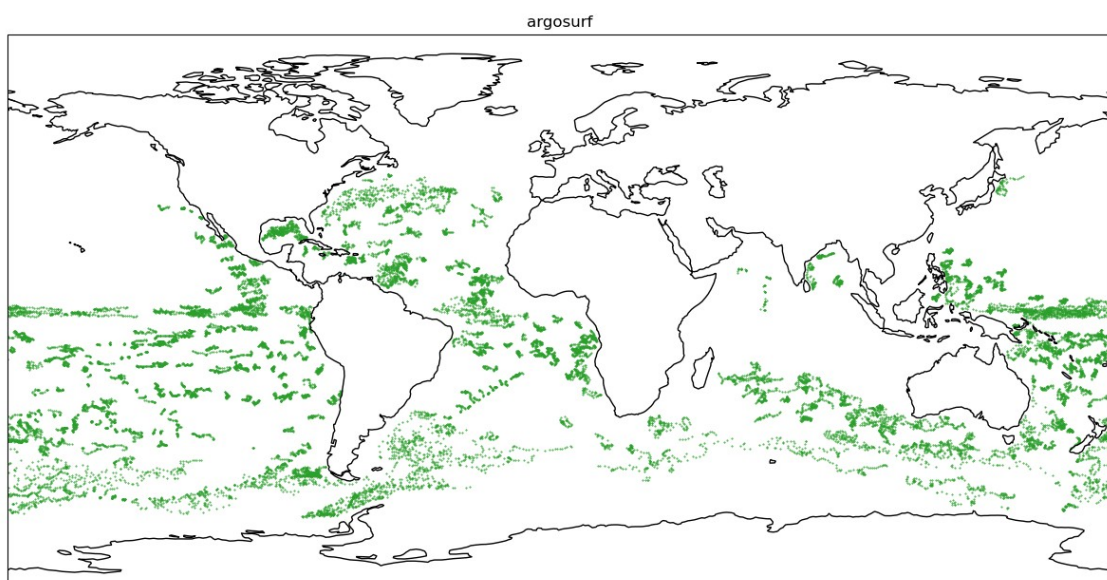
<sup>4</sup> For a full list of participating VOSclim ships, and supplementary information, see <http://lwf.ncdc.noaa.gov/oa/climate/vosclim/shipinfo.html> [last accessed 22<sup>nd</sup> April, 2024].



The ARGO surface dataset consists of a subset of the ARGO network, when the profiles also measure at depths shallower than 4m and up to 1 m. Both ARGO and ARGO surface data are obtained through the HadIOD.1.2.0.0 database<sup>5</sup> and are presented in Atkinson et al., 2014.



**Figure 8.** Geographical distribution of the Argo floats.



**Figure 9.** Geographical distribution of the surface Argo floats (bottom).

<sup>5</sup> Access to the HadIOD.1.2.0.0 User Guide at [https://www.metoffice.gov.uk/hadobs/hadiod/HadIOD.1.2.0.0 Product User Guide \[1.2\].pdf](https://www.metoffice.gov.uk/hadobs/hadiod/HadIOD.1.2.0.0%20Product%20User%20Guide%20[1.2].pdf) [last accessed April 10th, 2024].



## 2.5 Near-surface air temperature measurements for IST validation

Near-surface air temperature observations were used to validate the IST values in the product. The temperature observations come from three sources: the ECMWF (Section 2.5.1) CRREL (Section 2.5.2) and NP (Section 2.5.3), and comprise air temperatures measured at different heights (typically around 2 m above the surface) depending on e.g. snow accumulation, snow drift and snow melt. These temperature observations have been inspected and quality controlled manually for data artefacts. The ECMWF and CRREL observations have previously been used for validation of satellite ISTs and corresponding 2 m air temperature estimates within the European Union's Horizon2020 project EUSTACE (EU Surface Temperatures for All Corners of Earth; Nielsen-Englyst et al., 2021,2023; Rayner et al., 2020).

### 2.5.1 ECMWF distributed ice drifting buoys

Air temperature data from 116 drifting buoys were obtained from the Meteorological Archival and Retrieval System (MARS)<sup>6</sup> at the European Centre for Medium-Range Weather Forecasts (ECMWF), in 2015<sup>7</sup>. The temporal coverage is the period from 1993 to 2015, and the measurements are used for validation of the IST component (hereafter these data are referred to as “ECMWF buoys”).

### 2.5.2 CRREL mass balance buoys

These air temperature measurements were obtained using U.S.Army Cold Regions Research Engineering Laboratory (CRREL) mass balance buoys over the period 2001–2017 (Perovich et al., 2016; Richter-Menge et al., 2006).

### 2.5.3 NP drifting ice stations

This set of air temperature measurements were obtained by 14 Russian North Pole (NP) drifting ice stations mainly over the period 1982–1989 but also some for the period 2003–2012 (RU/FSR/HME/AARI and NSIDC, 1993).

<sup>6</sup> See <https://www.ecmwf.int/en/forecasts/access-forecasts/access-archive-datasets> [last accessed January 1st, 2024]

<sup>7</sup> Retrieving air temperature data from the MARS system is not immediately intuitive. For users interested in accessing their own set of data, our settings were set such that STREAM = OPER, TYPE = OB, CLASS = OD, REPRES = BU, OBSGROUP = CONV, EXPVER = 0001, TIME = 0000, RA = 86399, OBSTYPE = 11/13/19/21/180/181/182/183, TARGET = ecm-obsdata\_{\$startdate}-{\$enddate}\_{\$area\_n}\_{\$area\_w}\_{\$area\_s}\_{\$area\_e}, EXPECT = ANY, DUPLICATES = KEEP, DOMAIN = G, PADDING = 0, AREA = \$area\_n/\$area\_w/\$area\_s/\$area\_e, DATE = \$startdate/to/\$enddate.

A one-line command was executed on the bufr dump from MARS, “dbamsg dump <bufr-file-from-MARS> > <output-file>”. The information from the <output-file> was then transferred to a text file, which was split into separate files for each observation platform id. These were then saved in netcdf format. Finally, they were quality controlled using a visual inspection before they were used for validation. Note that at the time of this document’s publishing, researchers at DMI are working on updating these to get data after 2015 for validation of the C3S L4 SST/IST product.



### 2.5.4 SIMB3 buoys

Air temperature measurements are also used from all available Seasonal Ice Mass Balance Buoy 3 (SIMB3) from the Cryosphere Innovation. This is a four-season, autonomous, platform for in-situ observation of sea, lake, and pond ice. Developed for use in the high-Arctic, it is a 4.5m long buoy allowing remote monitoring of floating ice and collects a suite of data, e.g. ice thickness, growth, and melt. Data are available immediately after transmission via a real-time data portal. See <https://www.cryosphereinnovation.com/docs/simb3-introduction> for further information<sup>8</sup>.

The temperature observations from the SIMB3 buoys are air temperatures measured at different heights (typically around 2 m above the surface) depending on e.g. snow accumulation, snow drift and snow melt.

### 2.6 IceBridge Flights

Ice surface measurements from the skin layer of ice are used from the IceBridge Flights datasets. This dataset consists of more than hundred NASA IceBridge (IAKST1B) flights covering the period 2012–2019 (version 2; Studinger, 2020). The flights are typically conducted during March–May and the surface temperatures are converted from IR radiation measurements from a Heitronics KT-19 IR Radiation Pyrometer (assuming an emissivity constant of 0.97). The ISTs provided by IceBridge are at a spatial resolution of about 15m, and for validation purposes they have been averaged for every 5 km to remove the small-scale variability, which cannot be represented by the coarser resolution L4 IST product.

## 3. Description of product validation methodology

An assessment of product quality will examine three aspects of the data products:

1. The SST and IST values,
2. The SST uncertainty, and IST uncertainty values,
3. The stability of the SST and IST CDR and ICDR records.

Match-up datasets containing coincident in situ observations and the satellite observations of the L4 SST/IST product were created for each type of reference observation and each component of the L4 product, separately.

### 3.1 Validation of SST and IST

The L4 SST and IST fields will be validated separately using the independent in situ observations listed in Section 2. The differences between the L4 SST/IST and reference data are analysed using robust statistics, i.e. that are less influenced by outliers in the distribution of differences.

Outliers arise in both satellite and validation data, and robust statistics better describe the majority of data that are more normally distributed. The measures used here are the median and the robust standard deviation (RSD) given by 1.4826 times the median absolute deviation.

<sup>8</sup> <https://www.cryosphereinnovation.com/docs/simb3-introduction> [last accessed 20th June 2024].



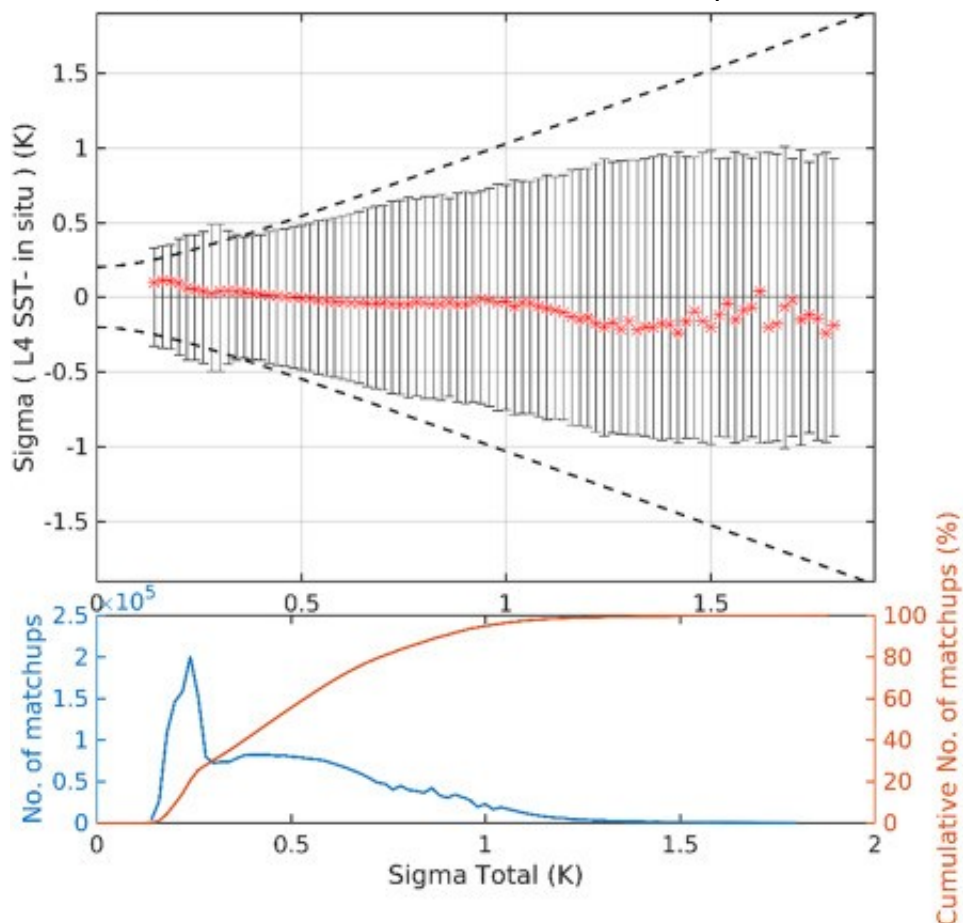
Satellite and reference datasets are compared using global statistics, time-series and spatial maps.

For the SST component, direct comparison of the SST value with in situ measurements from the sources described in section 2 is to be performed. For the IST component, as most in situ observations are from 2m air temperatures, comparison of the IST value with the 2m air temperature is performed. When direct skin measurements are available, i.e. from the IceBridge flights, IST is compared to skin surface temperature.

### 3.2 Validation of uncertainties

For SST, the uncertainty validation approach is similar to that done by Alerkans et al. (2020) and Nielsen-Englyst et al. (2018, 2023). An example output is shown in Figure 10, where the dashed lines represent the ideal uncertainty based on the assumption that drifters have a total uncertainty of 0.2 K (Kennedy, 2014).

This approach is unfortunately not applicable for the IST validation results due to the lack of good quality in situ reference observations, that makes the spatial sampling component very large in comparisons between the L4 IST and the in situ measured near-surface air temperatures. However, using the SIMB3 stations, the modelled uncertainties of the IST component will be assessed.



**Figure 10.** Typical uncertainty validation plot from Nielsen-Englyst et al. (2023). Along the x-axis is the estimated uncertainty which is calculated as part of the Optimal Interpolation (OI). The y-axis represents the standard deviation between the L4 SST and in situ measurement, which will be affected by errors in both the



satellite and in situ observations. The dashed lines show the ideal uncertainty when accounting for uncertainties in the drifter SSTs and the sampling error. The solid black lines show one standard deviation of the L4 SST minus drifter SST differences for each 0.02 K bin and the red asterisks mark the mean difference. The bottom plots show the number of matchups (blue) and the cumulative percentage of matchups for each bin (red).

### 3.3 Stability assessment

Based on the expected magnitude of a climate change signal (per decade), the requirements of an SST CDR are an accuracy of 0.1 °C and a stability (per decade) of 0.04 °C according to Ohring et al. (2005). For the Ice Surface temperature, which is also an ECV according to GCOS (since 2022), the CDR requirements are 0.3 °C/decade for the threshold stability and 0.1 °C/decade for the target stability (GCOS, 2022). Both metrics are calculated at a global level using in situ observations as the reference, drifting buoys for the SST component and sea ice buoys and drifting stations for the IST component according to Ohring et al. (2005).

## 4. Summary of validation results

Initial results are not available as the L4 SST/IST CDR has not been produced due to the unavailability of upstream input data at the time of writing this document, i.e. the ESA CCI v3.0 L3U dataset has not been released yet.

Detailed results will be available in the Product Quality Assessment Report [D1] when it is made available.



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