



Algorithm Theoretical Basis Document (ATBD)

Global L4 Sea and Sea-Ice Surface Temperature (SST/IST) Climate Data Record, Version 1.0

WP2-FDDP-SST/IST-v1.0

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History of document modifications

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1.1	25/11/2024	Document amended to account for feedback from independent review	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	Global L4 Sea and Sea-Ice Surface Temperature (SST/IST) Climate Data Record	CDR	1.0	15/12/2024
WP2-ICDR-SST-v1.0	Global L4 Sea and Sea-Ice Surface Temperature (SST/IST) Interim Climate Data Record	ICDR	1.0	15/12/2024



Related documents

Reference ID	Document
D1	Embury et al. (2023) ESA CCI Phase 3 Sea Surface Temperature (SST): Algorithm Theoretical Basis Document. European Space Agency contract no. ESA/AO/1-9322/18/I-NB. Document Ref. ESA SST_CCI_D2.1_ATBD_v3.1. Available at: https://climate.esa.int/media/documents/SST_CCI_D2.1_ATBD_v3.1-signed.pdf [last accessed 8 th October, 2024]
D2	GHRSSST data specification (GDS) 2.1 version 0; https://zenodo.org/records/6984989
D3	Karagali, I. et al. (2024) Global L4 Sea and Sea Ice Surface Temperature Climate Data Record, Version 1.0: Product User Guide and Specifications. Copernicus Climate Change Service. Document ref. C3S2-312b_WP2-FDDP-SST/IST_2024_PUGS_v1.1.
D4	Høyer et al. (2019) ESA SST CCI Phase-II Passive Microwave SST Production and Impact Assessment. European Space Agency. Document Ref. SST_CCI-WP90-DMI-201. Available at: https://climate.esa.int/media/documents/SST_CCI-WP90-Final_Report_Issue-1_signed.pdf [Last accessed 8 th October, 2024]
D5	Karagali, I. et al. (2024) Global L4 Sea and Sea Ice Surface Temperature Climate Data Record, Version 1.0: Product Quality Assessment Report. Copernicus Climate Change Service. Document ref. C3S2-312b_WP2_FDDP-SST/IST_2024_PQAR_v1.X. -
D6	Karagali, I. et al. (2024) Global L4 Sea and Sea Ice Surface Temperature Climate Data Record, Version 1.0: Target Requirements and Gap Analysis Document. Copernicus Climate Change Service. Document ref. C3S2_312b_WP3-TRGAD_SST/IST_v1.2 ¹
D7	Eastwood, S. and Dybkjaer, G. (2024) Sea Ice Surface Temperature, Version 1.1: Product User Guide and Specification. Copernicus Climate Change Service. Document ref. WP2_FDDP-SI-IST-v1.1_C3S2_MOI_PUGS-of-v1.0-IST-products_v1.X ²
D8	Eastwood, S., Dybkjaer, G., and Howe, E. (2023) C3S Sea Ice Surface Temperature Version 1.0: Algorithm Theoretical Basis Document. Copernicus Climate Change Service, Document ref. WP2_FDDP-SI-IST-v1.0_C3S2_ATBD-of-v1.0-IST-products_v1.1.

¹ Note this ATBD describes a product developed in an effort to address gaps identified by this 2024 Target Requirements and Gaps Analysis Document (TRGAD). There may be more recent TRGAD documents available on the CDS, that users may find useful if they wish to stay updated on the latest state-of-the-science.

²Users should consult the latest version of the PUGS available.



Acronyms

Acronym	Definition
AMSR-E	Advanced Microwave Scanning Radiometer for the Earth Observing System
AMSR2	Advanced Microwave Scanning Radiometer 2
ATSR	Along Track Scanning Radiometer
ATBD	Algorithm Theoretical Basis Document
AVHRR	Advanced Very High Resolution Radiometer
AASTI	Arctic and Antarctic Ice Surface Temperatures from AVHRR
CARRA2	Copernicus Arctic Regional Reanalysis 2nd generation
C3S	Copernicus Climate Change Service
CCI	Climate Change Initiative
CDR	Climate Data Record
CDS	Climate Data Store
CEDA	Centre for Environmental Data Analysis
DMI	Danish Meteorological Institute
DMI-MS-C-SIC	Danish Meteorological Institute's Multi-Sensor Composite of Sea Ice Concentration data
ECMWF	European Centre for Medium-Range Weather Forecasts
ESA	European Space Agency
EUMETSAT	European Meteorological Satellites
EPS	EUMETSAT Polar System
ERS	European Remote Sensing
EOCIS	UK Earth Observation Climate Information Service
FMI	Finnish Meteorological Institute
GAC	Global Area Coverage
GCOM	Global Change Observation Mission
GDS	GHRSSST Data Specification
GHRSSST	Group for High Resolution SST
ICDR	Interim Climate Data Record
TIR	Thermal Infrared
IST	Sea Ice Surface Temperature
JAXA	Japan Aerospace Exploration Agency
LECT	Local Equator Crossing Time
L2P	Level-2 Pre-processed data product
L3	Level-3 data product
L3C	Level-3 Collated data product
L3U	Level-3 Uncollated data product
L4	Level-4 data product
MCAS	Marine and Climate Advisory Service
MIZ	Marginal Ice Zone
MetNo	Norwegian Meteorological Institute
NASA	National Aeronautics and Space Administration



NP	North Pole
NOAA	National Oceanographic and Atmospheric Administration
NWP	Numerical Weather Prediction
OSI SAF	Ocean and Sea Ice Satellite Application Facility
OI	Optimal Interpolation
PMW	Passive Microwave
POES	Polar Operational Environmental Satellites
RDAC	Regional Data Assembly Centre
R&D	Research and development
SI	Sea Ice
SIC	Sea-ice concentration
SMHI	Swedish Meteorological and Hydrological Institute
SLSTR	Sea and Land Surface Temperature Radiometer
SST	Sea Surface Temperature
TB	Brightness Temperature
USNIC	U.S. National Ice Center
UISST	Under-ice SST



General definitions

Climate Data Record (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.

Interim Climate Data Record (ICDR) - 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.

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

Sea Surface Temperature (SST) – the temperature of the ocean water close to the surface.

SST_{20cm} – 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.

Sea Ice Surface Temperature (IST) – representative of the surface temperature over 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).

Marginal Ice Zone (MIZ) – Marginal Ice Zone, a part of the seasonal ice zone that varies in width (100 to 200 kilometres) 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.



Level-2 Pre processed (L2P) data product – Geophysical variables derived from Level 1 source data on the Level 1 grid (typically the satellite swath projection). Ancillary data and metadata added following GHRSSST Data Specification.

Level-3 Uncollated (L3U) data product – 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.

Level-3 Collated (L3C) data product – 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.

Level-3 Super-Collated (L3S) data product – 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.

Level 4 (L4) data product – SST observations from multiple instruments using an analysis system (e.g. optimal interpolation) to produce a gridded, gap-free product.



Table of Contents

History of document modifications	3
List of datasets covered by this document	3
Related documents	4
Acronyms	5
General definitions	7
Scope of the document	10
1. Executive summary	10
2. Instruments	12
2.1 Advanced Very High Resolution Radiometers (AVHRRs)	12
2.2 Along Track Scanning Radiometer (ATSR)	13
2.3 Sea Land Surface Temperature Radiometer	14
2.4 Advance Microwave Scanning Radiometer (AMSR-E)	14
2.5 Advance Microwave Scanning Radiometer 2 (AMSR2)	14
3. Input and auxiliary data	15
3.1 SST CCI CDR	15
3.2 SST ICDR	16
3.3 IST AASTI CDR + C3S ICDR	16
3.4 Sea Ice Concentration data	16
3.5 Land Mask	17
4. Algorithms	18
4.1 Pre-processing of input data.	18
4.2 Surface Mask	19
4.3 Optimal Interpolation (OI) Method	20
4.3.1 Statistical inputs	20
4.4 Post-Processing	20
5. Output data	23
5.1 File format and naming scheme	23
5.1.1 Date	23
5.1.2 Time	23
5.1.3 Dataset.....	23
5.2 File contents	24
References	25



Scope of the document

This document is the Algorithm Theoretical Basis Document (ATBD) for the L4 SST/IST CDR, version 1.0, produced by DMI. This document describes the algorithm used to generate the L4 product, including the scientific justification for the algorithm selected to derive the product, an outline of the approach used, a listing of the assumptions and limitations of the algorithm, and a brief overview of the final product (more detailed information on the Product specifications can be found in [D3]).

1. Executive summary

This document presents the algorithm, input and auxiliary data used in the production of the global Level 4 Sea and Sea-Ice Surface Temperature Climate Data Record (CDR) and additional Interim CDR products (ICDR), generated by the Danish Meteorological Institute. This product is the first global CDR to combine surface temperatures acquired over the open ocean (SST), the marginal ice zone (MIZ) and sea-ice (IST), into a single product. The Copernicus Climate Change Service (C3S) ICDR is intended to be used in combination with the corresponding C3S CDR.

Both the L4 SST/IST CDR and ICDR are produced using SST (adjusted to a daily mean temperature at 20cm depth to allow comparison with the historical in situ record) from the European Space Agency (ESA) SST_cci CDR single-sensor Level 3 Uncollated (L3U) datasets and an associated ICDR whose production was funded through the C3S (2022) and the EOCIS/MCAS (from 2023 onward). The IST inputs, representing the skin surface temperature of the sea ice, are from the C3S L3 SI-IST CDR/ICDR v1.1.

The CDR is generated using input data from the various sensors. For the SST, Level 3 data from the Along Track Scanning Radiometer (ATSR), Advanced Very-High Resolution Radiometer (AVHRR), Sea Land Surface Temperature Radiometer (SLSTR) and Level 2P data from the Advance Microwave Sensing Radiometer 2/E are used; these have been generated by the ESA SST_cci. For the Ice Surface Temperature (IST) component, the Arctic and Antarctic Ice Surface Temperatures from thermal Infrared satellite sensors (AASTI) baseline CDR v1.1 (1982-2019 June), brokered by DMI and MetNo and its extension, the ICDR v1.1 (July 2019 onward), produced by C3S are used. Only L2P AVHRR data are used for the production of the L3 IST CDR and ICDR.

The ICDR is generated using SST input from Level 3 Advanced Very-High Resolution Radiometer (AVHRR) and Level 3 Sea Land Surface Temperature Radiometer (SLSTR) products. For the IST component, the C3S L3 SI-IST ICDR v1.1 is used.

Both ICDR and CDR datasets are generated using the same software and algorithm originally developed within the MyOcean project and currently applied to the operational Multi-Year products for the SST and IST delivered to the Copernicus Marine Service. The main frame of the processing algorithm relies on (i) generating an aggregated observational field from the single sensor input data, and (ii) implementing an Optimal Interpolation algorithm to fill in the gaps from missing data.



The data records consist of daily L4, gridded surface temperature fields covering the period from 1982 to end-2021 for the CDR; while the ICDR provides an ongoing extension in time of the record from Jan 2022 onwards. Two temperature fields are provided in the data product: (i) the main SST/IST field, with a coupled uncertainty estimate, and (ii) a second SST-only field with an uncertainty estimate, which includes an estimate of surface water temperature underneath the sea-ice in the place of Sea Ice Surface temperatures.

The document is structured as follows. Section 1 gives an overview of the instruments used to collect the raw measurements. Auxiliary datasets used in the processing are then described in Section 2. Section 3 provides a detailed description of the algorithm used to produce the L4 data, while Section 4 provides some overview information on the product itself including information on formats, specifications (note that more detailed product specification information can be found in the Product User Guide and Specifications document [D3]).



2. Instruments

The SST/IST v1.0 product is generated using measurements from a range of Infrared and Microwave sensors. Five sensor lineages have been used to produce this Climate Data Record. Overviews of each instrument are provided here, while Sections 3.1 to 3.3 highlight which sensors specifically contribute to the generation of the SST and IST elements of the product.

2.1 Advanced Very High Resolution Radiometers (AVHRRs)

The Advanced Very High Resolution Radiometers (AVHRRs) are a series of multipurpose imaging instruments carried onboard the National Oceanic and Atmospheric Administration (NOAA) Polar Operational Environmental Satellites (POES) and EUMETSAT Polar System (EPS) MetOp satellites. As of 2024 there are 4 AVHRR instruments still in operation. The AVHRR is an across-track scanning radiometer using six spectral channels (early versions of the instrument had four or five channels), with a spatial resolution of approximately 1.1 km at nadir. There are 2048 pixels in each scan for a swath width of about 2800 km. Due to hardware limitations upon the original design, recording a complete orbit of full resolution data for transmission to the ground station was not possible. Therefore, the onboard processor samples the real-time data to produce reduced resolution Global Area Coverage (GAC) data with a nominal resolution of ~4km. The more recent MetOp satellites do not have this limitation and record full orbit data at native resolution.

The list of platforms carrying AVHRR instruments data of which are used in the production of the L4 SST/IST CDR/ICDR are listed in Table 1.

Table 1. List of platforms carrying AVHRR instruments, data from which are used in the L4 SST/IST CRD/ICDR.

Satellite	Type	Overpass Time	Operations start	Operations end
NOAA-6	AVHRR/1	AM	Jul 1979	Mar 1982
NOAA-7	AVHRR/2	PM	Sep 1981	Feb 1985
NOAA-8	AVHRR/1	AM	May 1983	Oct 1985
NOAA-9	AVHRR/2	PM	Feb 1985	Nov 1988
NOAA-10	AVHRR/1	AM	Nov 1986	Sep 1991
NOAA-11	AVHRR/2	PM	Nov 1988	Dec 1994
NOAA-12	AVHRR/2	AM	Sep 1991	Dec 1998
NOAA-14	AVHRR/2	PM	Jan 1995	Oct 2002
NOAA-15	AVHRR/3	AM	Oct 1998	Dec 2010
NOAA-16	AVHRR/3	PM	Jan 2001	Dec 2010
NOAA-17	AVHRR/3	AM	Jun 2000	Dec 2010
NOAA-18	AVHRR/3	PM	May 2005	Ongoing
MetOp-A	AVHRR/3	AM	Oct 2006	Nov 2021
NOAA-19	AVHRR/3	PM	Feb 2009	Ongoing
MetOp-B	AVHRR/3	AM	Jan 2013	Ongoing
MetOp-C	AVHRR/3	AM	Jan 2019	Ongoing



2.2 Along Track Scanning Radiometer (ATSR)

The Along Track Scanning Radiometers (ATSR) instruments are well calibrated, dual-view radiometers intended to produce long-term, consistent SST observations. Three ATSR instruments have flown on board ESA's two European Remote Sensing (ERS) satellites and ENVISAT satellite. All three satellites were in stable sun-synchronous orbits with near-constant Local Equator Crossing Times (LECTs) – the ERS-1 and ERS-2 platforms had a LECT of 10:30 and ENVISAT had a crossing time of 10:00 all of which were maintained within a few minutes.

The ATSR instruments had four key design features making them better suited to climate applications than the AVHRR instruments:

1. The instrument spectral response functions were accurately measured during pre-flight calibration and characterisation.
2. The ATSRs were exceptionally well calibrated with two accurate onboard calibration targets at temperatures of ~ 260 K and 300 K which greatly reduced non-linearity errors for ocean observations (for comparison AVHRR instruments have a single on-board target at ~ 290 K and rely on a space view (2.7 K) to provide the second point).
3. The infrared detectors were actively cooled to ~ 82 K to reduce instrument noise and avoid temperature dependent effects on calibration. In addition, the instrument fore-optics were cooled below ambient temperature to reduce self-emission issues, and the instrument was enclosed to prevent stray-light affecting the detectors.
4. The dual-view capability using a single telescope with a conical scanning pattern provided both a nadir-view and an inclined forward view ($\sim 55^\circ$). Having two views of the Earth's surface allowed the instrument to gather more information and more effectively separate surface and atmospheric effects; i.e. the SST retrieval could be made more robust to atmospheric conditions, including water vapour and stratospheric aerosol.

The first ATSR carried onboard ERS-1 was a four-channel radiometer with channels at 1.6, 3.7, 11, and 12 μm . However, the ATSR-1 instrument would only transmit one of the 1.6 or 3.7 μm channels with the selection based on the 1.6 μm reflectance intended to separate day and night-conditions. There were two major issues affecting the ATSR-1 instrument:

1. The 3.7 μm channel failed in May 1992, less than a year after the satellite was launched
2. In order to preserve mission lifetime the temperature of the actively cooled detectors were allowed to rise, by-end of mission the detectors were operating at over 110 K.

The second ATSR carried onboard the ERS-2 added three reflectance channels at 0.55, 0.67, and 0.87 μm mainly for vegetation monitoring. The channels had only limited availability over ocean due to telemetry bandwidth limitations; depending on instrument operating mode the visible channels may be transmitted for a reduced narrow swath, reduced 8-bit digitization, or interlaced (record every-other) pixels. The final, Advanced ATSR, instrument onboard ENVISAT was functionally the same as ATSR-2 but without the bandwidth limitations so all seven channels are always available in full resolution.



2.3 Sea Land Surface Temperature Radiometer

The Sea Land Surface Temperature Radiometer (SLSTR) instrument is a well calibrated, dual-view radiometer intended to produce long-term, consistent SST observations. The design of the SLSTR instrument builds on the heritage of the earlier (A)ATSR instruments adding more spectral bands and a wider swath. The first SLSTR instrument is carried onboard the Sentinel-3A satellite launched in February 2016, with the second Sentinel-3B was launched in April 2018.

2.4 Advance Microwave Scanning Radiometer (AMSR-E)

The Advanced Microwave Scanning Radiometer for EOS (AMSR-E) is a twelve-channel, six-frequency microwave radiometer supplied by the Japan Aerospace Exploration Agency (JAXA) for the National Aeronautics and Space Administration's (NASA's) Earth Observation System Aqua platform. It measures brightness temperatures at 6.9, 10.7, 18.7, 23.6, 36.5 and 89.0 GHz at both horizontal and vertical polarization and at an Earth incidence angle of approximately 55 degrees. A 1.6 meter offset parabolic reflector antenna collects the microwave radiation and results in spatial resolutions ranging from approximately 56 km at 6.9 GHz to approximately 5 km at 89.0 GHz. The 89.0 GHz channels are sampled every 5 km, all other channels every 10 km. The dataset used in the present study consists of spatially re-sampled brightness temperatures at the resolution of the 6.9 GHz channel (Ashcroft and Wentz, 2013) and covers the period June 2002 to October 4, 2011. For further information on the production of SST and impact assessment see [RD4].

2.5 Advance Microwave Scanning Radiometer 2 (AMSR2)

The Advanced Microwave Scanning Radiometer 2 (AMSR2) is an instrument on JAXA's Global Change Observation Mission 1st – Water (GCOM-W1) platform. GCOM-W1 was launched in May 2012 and began collecting data on July 4, 2012. AMSR2 measures brightness temperatures at 6.9, 7.3, 10.7, 18.7, 23.6, 36.5 and 89.0 GHz at both horizontal and vertical polarization and at an Earth incidence angle of approximately 55 degrees. Note the addition of the 7.3 GHz channels relative to AMSR-E, added for RFI mitigation. AMSR2 uses a 2 meter offset parabolic antenna to obtain a spatial resolution ranging from 4 km at 89.0 GHz to approximately 45 kilometres at 6.9 and 7.3 GHz. The 89.0 GHz channels are sampled every 5 km, all other channels every 10 km. We use the dataset of Brightness Temperature Modified Using the Antenna Pattern Matching Technique (Maeda et al., 2016) which contains similar spatially resampled brightness temperatures to the AMSR-E dataset. For further information on the production of SST and impact assessment see [RD4].



3. Input and auxiliary data

The basic input and auxiliary data used for the global SST/IST L4 product are described in more detail below. All input data are pre-processed and re-projected (when required) to match the target grid of the L4 SST/IST CDR/ICDR product, i.e. global at 0.05 degrees. An overview is provided in Figure 1.

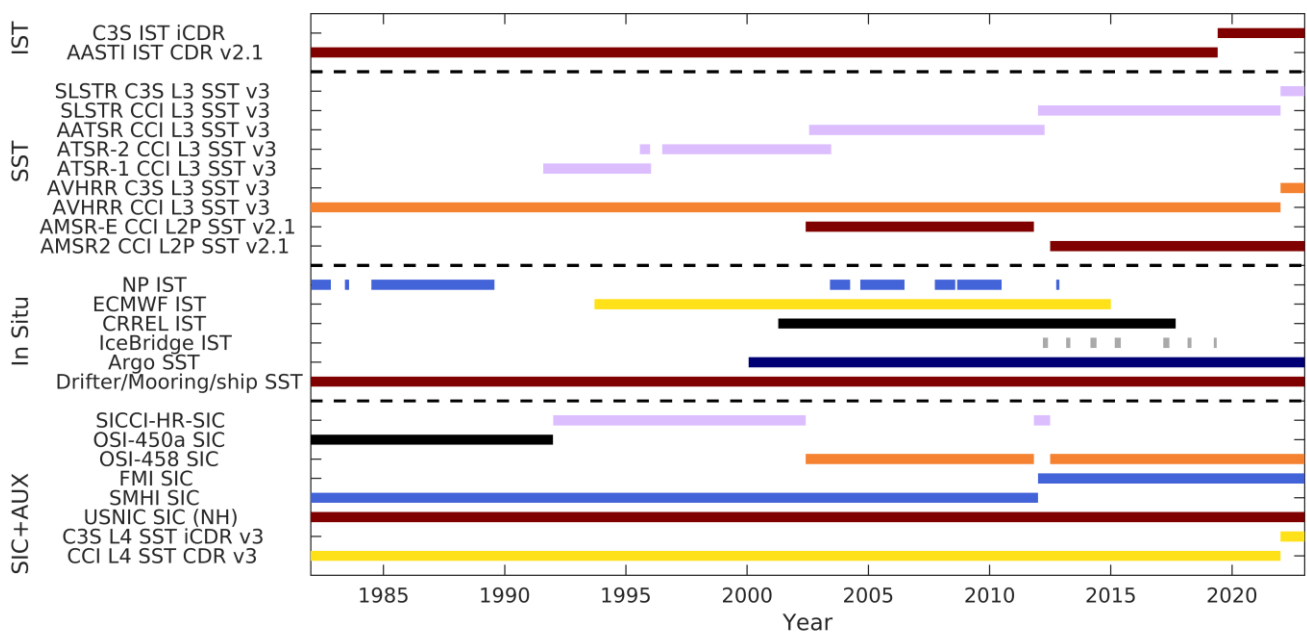


Figure 1. Overview of input data (including product level L3 or L2P), auxiliary data and in situ data used for the validation along with the CDR / ICDR (dark red) datasets.

3.1 SST CCI CDR

Single-sensor L2P and L3U SST data from version 3 of the Climate Data Record (CDR) produced by the European Space Agency (ESA) Climate Change Initiative Sea Surface Temperature project (ESA SST_cci Version 3.0, <http://cci.esa.int/>, [D1]) are used for the period January 1982 to December 31st, 2021 (Embury et al., 2024). The CDR accurately maps the sea surface temperature of the global oceans over the period 1980 to 2021 using observations from many satellites, with a high degree of independence from in situ measurements. The data provide independently quantified SSTs to a quality suitable for climate research. The selected fields are the sea surface temperature retrievals at 20 cm depth. The ESA CCI data series include observations from the ATSR 1 instrument on board the ERS-1 satellite (L3U), ATSR 2 on board the ERS-2 satellite (L3U), the AATSR on board ENVISAT (L3U), AVHRR onboard the NOAA and MetOp satellites (L3U), SLSTR on board Sentinel-3 A/B (L3U), AMSR2 onboard the GCOM-W1 platform and AMSRE on Aqua (L2P). Further detailed information on how these input data are produced can be found in [D1].



3.2 SST ICDR

Single-sensor L3U SST data from 2022 onwards are provided as an Interim Climate Data Record (ICDR) and are updated daily at one month behind present. The Copernicus Climate Change Service (C3S) funded the development of the ICDR extension and production of the ICDR during 2022. From 2023 onwards the production of the ICDR is funded by the UK Earth Observation Climate Information Service (EOCIS) and Marine and Climate Advisory Service (MCAS). The selected fields are sea surface temperature depth retrievals representative of the SST at 20 cm depth. The ICDR includes observations from the SLSTR A/B instruments on board the Sentinel 3 satellites (L3U) and the AVHRRs on board the NOAA and MetOp satellites (L3U).

3.3 IST AASTI CDR + C3S ICDR

The IST observations are obtained from the C3S L3 SI-IST CDR/ICDR v1.1 [D7, D8] which in itself consists of the Arctic and Antarctic Ice Surface Temperatures from thermal Infrared satellite sensors (AASTI) baseline CDR v1.1, for the period 1982-2019 (June), brokered by DMI and MetNo and its extension, the ICDR v1.1, from July 2019 and onward, produced by C3S. For the creation of this dataset, observations from the two Thermal Infrared (TIR) brightness temperature (TB) window channels from AVHRR 2/3 instruments on board all NOAA and MetOp satellites from the period covered are used (see Table 1). Due to direct access to the production chain of the C3S L3 SI-IST CDR/ICDR v1.1 and to ensure control of how the IST component is ingested in the DMIOI processing chain, the L2P files on which the C3S L3 SI-IST CDR/ICDR v1.1 is based, are used rather than the final L3 product. Note that this product only covers the south and north hemisphere polarward of 50°.

3.4 Sea Ice Concentration data

A new sea ice concentration (SIC) Multi-Sensor Composite (MSC) dataset produced for the Copernicus Arctic Regional Reanalysis 2nd generation (CARRA2) Pan-Arctic extension³ (referred to as DMI-MSC SIC) is used by the L4 analysis system for the northern hemisphere, while a rerun of the CARRA2 SIC processing has been produced for the southern hemisphere. The SIC dataset is a Multi-Source Composite (MSC) of SIC estimates, based on SIC information from the EUMETSAT Ocean and Sea Ice Satellite Application Facility (OSI SAF) and ESA CCI Sea Ice products combined with different sources of ice charts. Produced at DMI, it is referred to here as DMI-MSC-SIC. The following products are included in the SIC processing:

- i. The Ocean and Sea Ice Satellite Application Facility's (OSI SAF) global SIC CDR v3, OSI-450a, used for the period 1982 to 1991.
- ii. The ESA CCI Sea ice CDR, SICCI-HR-SIC, used from 1992 to 2002. This was also used to bridge the gap in the AMSR satellite record, which occurs between the end of AMSR-E operations in October 2011 and the beginning of AMSR2 operations in May 2012. OSI SAF's OSI-458 based on AMSR satellite record and used for the period from 2002 to 2020

³For more information on the CARRA2 Pan-Arctic extension of the sea ice concentration dataset, see: <https://climate.copernicus.eu/copernicus-arctic-regional-reanalysis-service> [last accessed 8th October, 2024].



- iii. A special rerun of OSI SAF's OSI-458 product, produced by the Norwegian Meteorological Institute (MET Norway: MetNo) to produce consistent sea ice fields after 2020.
- iv. U.S. National Ice Centre's (NIC) ice charts used to identify land fast ice and to filter spurious sea ice along coasts
- v. The Swedish Meteorological and Hydrological Institute (SMHI) and Finnish Meteorological Institute's (FMI) ice charts used for the Baltic region for the entire period
- vi. ESA CCI SST v3.0 CDR is used to filter spurious sea ice

The rationale behind using this multi-source SIC composite is to always use the most accurate SIC field available. Land spillover effects are more pronounced in the OSI-450a and SICCI-HR-SIC compared to OSI-458 which is based on the higher resolution AMSR-E/AMSR2 sensors. To improve OSI-450a/SICCI-HR-SIC and to increase the consistency of the full SIC record, a number of filters have been applied to the SIC products using information from the NIC ice charts and the CCI SST CDR. In addition, an inter-sensor bias correction has been applied to increase the consistency of the combined SIC product. All of OSI-450a, SICCI-HR-SIC and OSI-458 have challenges in coastal regions, and for the Baltic Sea, Kattegat Bay and the Skagerrak Strait high resolution SIC information is used from the Swedish Meteorological and Hydrological Institute (SMHI; 1982-2011) and 1 km SIC fields (2012-present), which are based on ice charts.

3.5 Land Mask

For the classification between ocean and land, the land mask developed in the European Space Agency (ESA) Climate Change Initiative (CCI) SST project⁴ as defined in Merchant et al. (2019) and Carrea et al. (2015) is used. Note that all rivers and lakes except the Caspian Sea are masked out and are thus not represented in the product.

⁴ For more information see: <https://climate.esa.int/en/projects/sea-surface-temperature/> [Accessed Feb 2024]

4. Algorithms

The algorithm documented here describes the steps followed to generate the L4 SST/IST product. The same algorithm is used for both the CDR and ICDR products. Figure 2 shows a schematic overview of the DMI Optimal Interpolation (DMIOI) system where all input data on surface temperatures over sea, sea ice and the marginal ice zone along with the input SIC fields and the land mask are combined into the final OI L4 product.

The final L4 analysis product is a merged and interpolated daily field with a 0.05° resolution in latitude and longitude, and covers both open ocean, sea ice and the Marginal Ice Zone (MIZ). The optimal interpolation method used to construct the merged and gap free SST/IST analysis is taken from the high latitude SST DMI processing scheme described in Høyer and She (2007); Høyer et al. (2014).

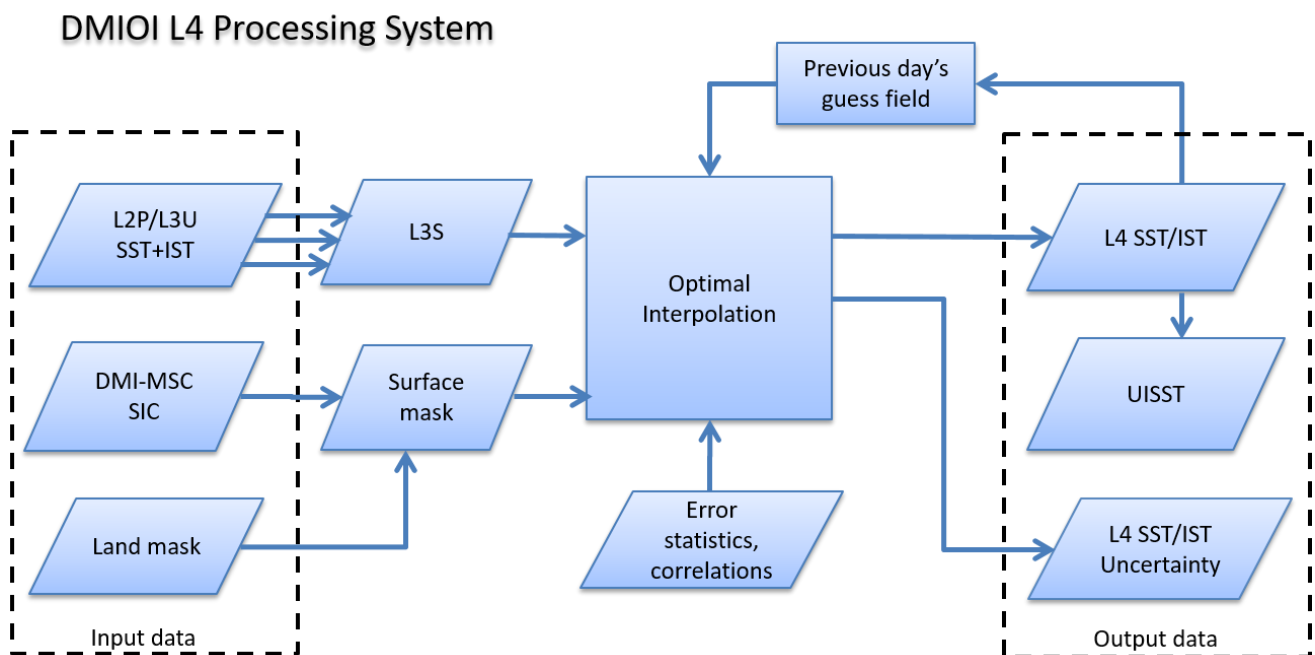


Figure 2. Schematic diagram of the DMIOI processing chain at DMI. Level 2 and Level 3 (L2P/L3) SST and IST data, Sea Ice Concentration data (DMI-MSC-SIC) and land/sea mask undergo a series of processes and finally an Optimal Interpolation methodology is applied to produce the Level 4 SST/IST data and its ancillary uncertainty dataset. An under-ice SST (UISST) is produced in the post-processing phase. Rectangles indicate processes, while slanted boxes indicate data products.

4.1 Pre-processing of input data.

The input L2P and L3U SST data undergo various QC and processing steps to generate separate single sensor level 3 collated products. The single sensor L3 collated fields are calculated as the average of all available observations (meeting the quality level requirement) within the aggregation window. The aggregation window is 24 h for most of the record, except from the period 1982-1986, when limited input observations are available, and the window has been extended to 60 h. Note the following:



- For SST from Infrared sensors, quality levels 4 and 5 are used.
- For SST from Passive Microwave, quality levels 3, 4 and 5 are used.

The input L2P IST data undergo the same QC and processing steps to generate single sensor level 3 collated fields, calculated as the average of all available observations meeting the requirement of quality levels 4 and 5, within the aggregation window (see above).

The L3S fields are calculated as a noise weighted average of all available observations within each grid cell.

4.2 Surface Mask

The input sea ice concentration field is combined with the land mask to generate a surface mask, which is used to characterise the surface type. Land points are assigned the value 2. For non-land points, depending on the sea ice concentration value ocean surface types are defined as open ocean (<15% sea ice concentration, assigned the value 1), marginal ice zone (15-70%) and sea-ice (>70%) surface are both assigned the value 9.

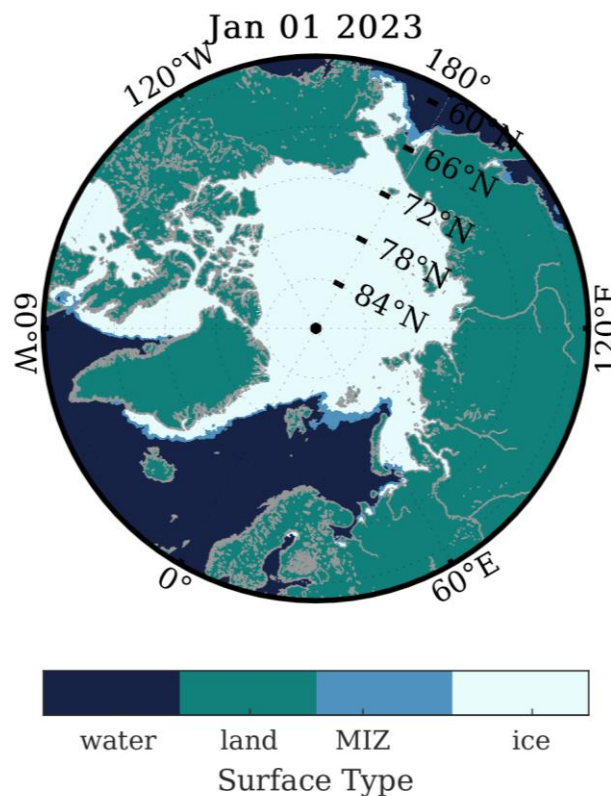


Figure 3. Example of surface mask for January 1st 2023 identifying the regions with open ocean (=1), land (=2), sea ice covered (=9) and Marginal Ice Zone (MIZ =9, defined as sea ice concentration between 15 and 70) for the Arctic Ocean.



4.3 Optimal Interpolation (OI) Method

The Optimal Interpolation (OI) method works with anomalies from a first guess field (Høyer and She, 2007). In the current approach, a persistence-based method is applied, which uses the previous day's analysis field as the first guess field (Nielsen-Englyst et al., 2023). The SST and IST observations from the last 24 hours are therefore interpreted as anomalies with respect to the first guess field, i.e. the previous day's analysis. For each grid point, the OI method finds the solution that has the lowest errors, with respect to given statistical inputs (such as a first guess error variance, error covariance functions and uncertainties on the individual observations). Due to the different physical conditions for ocean and sea ice surface temperature variability, separate statistics have been derived for the open ocean and the sea ice covered regions (see Section 4.3.1). The search radius for the OI method is set to 100 km and the maximum number of satellite observations included in the optimal estimation is 8. Each SST analysis value is accompanied by an uncertainty estimate which is an ancillary output of the Optimal Interpolation algorithm.

4.3.1 Statistical inputs

The SST and IST first guess variance and error covariance are derived from the observations. The first guess field and the error covariance used in the MIZ is a weighted linear combination of the open waters and the ice values, where the sea ice concentration is used as the weighting factor.

The correlation scales of the satellite anomalies have been derived empirically from observations. Spatially dependent error covariance functions have been fitted, based upon several years of analysis of level 3 SST and IST observations, separately for the SST, IST and the MIZ. These correlation scales comprise the "Error statistics, correlations" shown in Figure 2. The functions take the form of:

$$C_{ij} = \exp(-\lambda * dist_{ij}^{\gamma}) \quad [1]$$

where C_{ij} is the error covariance between two observations i and j , $dist_{ij}$ is the distance between the two observations, and λ and γ are the two parameters empirically determined from the observations that vary throughout the domain (see Nielsen-Englyst et al., 2023).

Note that grid points outside the sea ice grid or undefined within the sea ice grid use the SST statistics.

4.4 Post-Processing

The final L4 SST/IST field (see example in Figure 4, and 5b) is post-processed to generate an SST field, i.e. the field including only sea surface temperature which in sea-ice covered areas has a value representative of the water temperature below the ice (sub-ice SST or under-ice SST, UISST). This is shown in Figure 5a.

To estimate the field including only sea surface temperature, a salinity-based approach is used to calculate the freezing point temperature T_s , i.e. the temperature at which water freezes according to Banzon et al. (2020). The surface freezing temperature, T_f , was calculated using Millero's formula (Fofonoff and Millard, 1983) and the World Ocean Atlas 2018 salinity climatology (Garcia et al., 2019) and was further adjusted by a constant C and the sea ice concentration SIC , following the equation from Banzon et al. (2020):

$$T_{s(SIC)} = T_f + C(1 - SIC) \quad \text{for } 0 < SIC \leq 1. \quad [2]$$

An example of the two different fields (SST incorporating the UISST values, and the combined SST/IST field) can be seen in Figure 5.

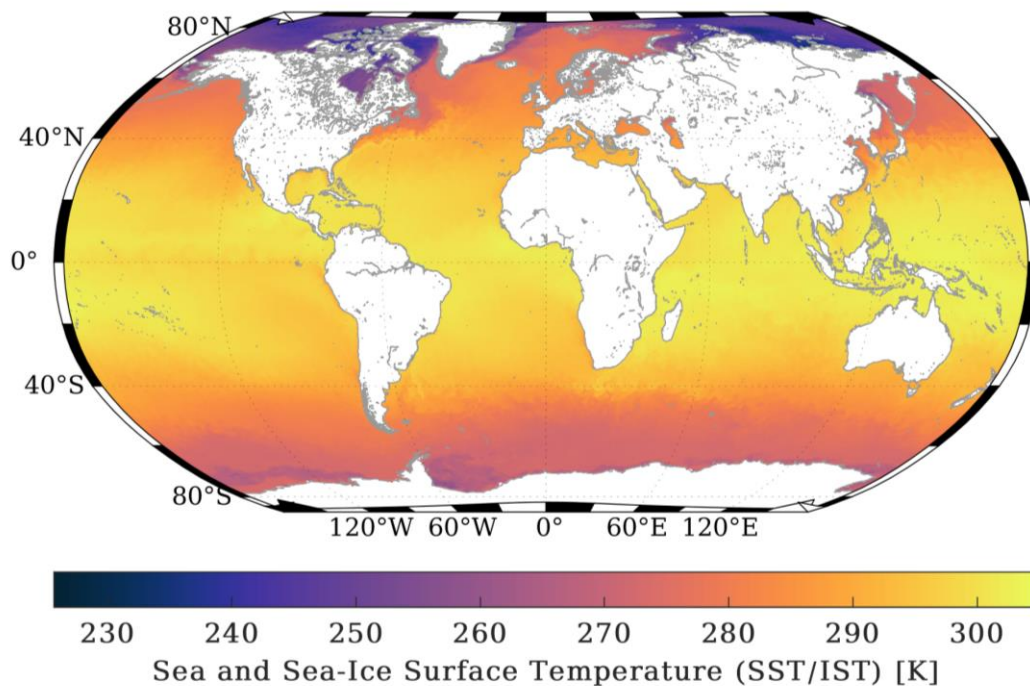


Figure 4. Example of the global final product including both sea surface and sea-ice surface temperatures for January 1st, 2023.

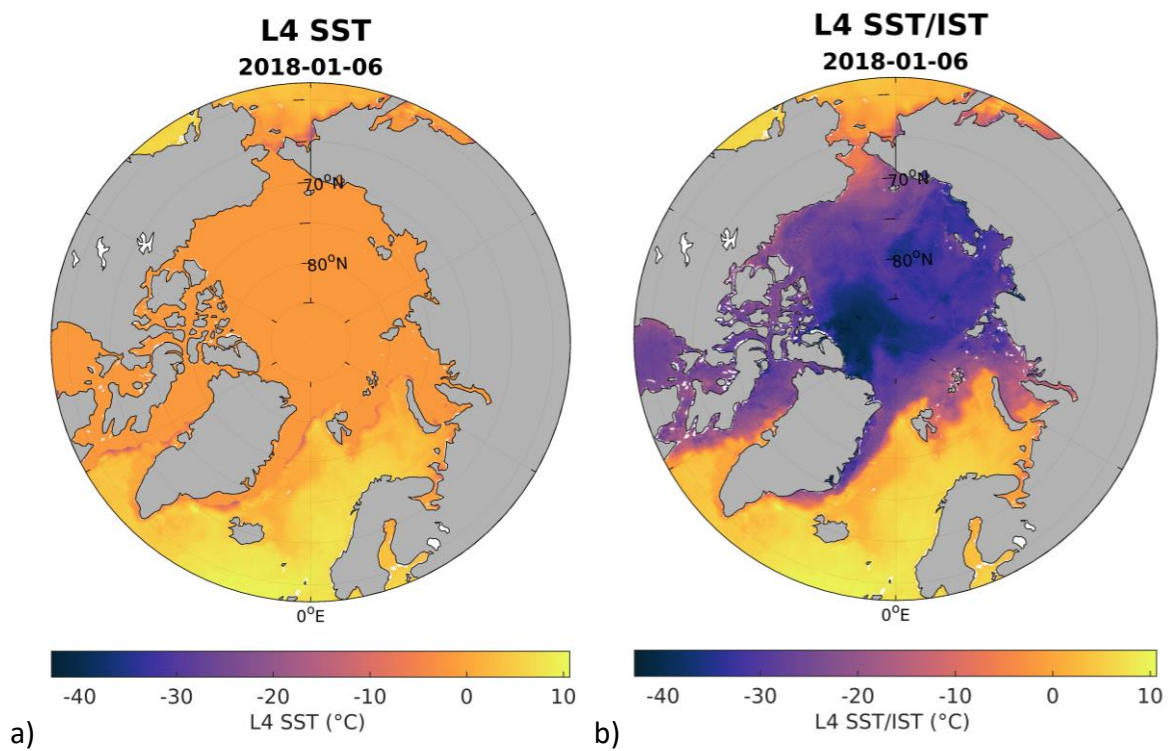


Figure 5. Example of the final product over the Arctic Ocean for SST and estimated Under-Ice SST (a) and combined SST and IST (b) fields in a single data product file (for data produced for the 6th January 2018).



5. Output data

5.1 File format and naming scheme

The output data are in netCDF4-classic format and follow the GHRSSST data specifications [D2]. The file names have the format:

```
<Date><Time>-C3S2-L4_GHRSSST-SSTdepth-ISTskin-DMIOI-GLOB_<Dataset>-v02.0-fv01.0.nc
```

The variable components within braces: <component> are summarised in Table 2 and detailed in the following sections. Note:

- <Dataset> corresponds to the GHRSSST <Additional Segregator> component and are therefore separated by an underscore (“_”) rather than a dash (“-”).
- The fixed version string “v02.0” indicates that the file is a GDS 2.0 format file. The Climate Data Record version is indicated by the <Dataset> string.

Table 2. GDS 2.0 file-naming convention components.

Component	Definition	Description
<Date>	YYYYMMDD	The identifying date for this file in ISO8601 basic format
<Time>	HHMMSS	The identifying time for this file in ISO8601 basic format
<Dataset>	CDR1.0 or ICDR1.0	Indicates if this file is CDR or ICDR and the version number; for L4 files this is prepended by ‘GLOB_’

5.1.1 Date

The identifying date for this file, using the ISO8601 basic format: YYYYMMDD.

5.1.2 Time

The identifying time for this file in UTC, using the ISO8601 basic format: HHMMSS. The time used for L4 files is the centre time of analysis window (120000 for daily files)

5.1.3 Dataset

Indicates which (Interim) Climate Data Record this file belongs to. Current strings in use are CDR1.0 ICDR1.0

L4 files include GLOB_ (i.e. GLOB_CDR1.0 or GLOB_ICDR1.0) to maintain the convention used for other files produced with the DMIOI system.



5.2 File contents

L4 files are supplied on a regular latitude/longitude grid (based on the WGS1984 geoid) and variables have dimensions:

- time: 1 (defined as unlimited)
- lat: Number of latitude points (3600)
- lon: Number of longitude points (7200)

Table 3. Main output variables included in the L4 files.

Variable name	Description
analysed_st	The temperature of the sea surface at 20cm, or sea-ice surface skin temperature, whichever is present at each location.
analysed_sst	The sea surface temperature over open ocean and under sea ice.
analysed_st_uncertainty	Uncertainty in the sea or sea ice surface temperature at each location.
analysed_sst_uncertainty	Uncertainty in the sea surface temperature (same as analysed_st_uncertainty) and the under-ice temperature.
sea_ice_fraction	Sea ice fraction at each location in the grid
mask	Information on whether is ocean, land, sea ice or marginal ice in each grid cell; set to 1 if the grid cell contains ocean; 2 for marginal ice zone (MIZ); 3 for sea-ice; 4 for lake and 8 for land.

Please note that the product mask's "lake" identifier refers only to the Caspian Sea. All other lakes are not represented and are thus classified as land in the dataset. Values in the mask variable can be used to identify only the ocean and Caspian Sea water grid points, sea-ice, land, and coastline.



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