

climate change initiative

SEA SURFACE TEMPERATURE A 42-year Sea Surface Temperature Climate Data Record from the ESA Climate Change Initiative Owen Embury, Chris Merchant, Simon Good, Jacob Høyer, Nick Rayner, Tom Block, Craig Donlon







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SST-CCI Climate Data Record v3

- ESA Climate Change Initiative (CCI) has produced two previous SST Climate Data Records (CDR):
 - Version 1: September 1991 December 2010 (19 years)
 - Version 2: September 1981 December 2016 (35 years)
- Version 3:
 - CDR: January 1980 December 2021 (42 years)
 - Interim-CDR (ICDR) 2022 to present at ~3 weeks latency

Improved AVHRR SST especially 1980s:

- Addition of AVHRR/1 from NOAA-6, -8, and -10
- Reduce 1980s data gaps
- Reduce desert-dust related biases
- New bias-aware optimal estimation retrieval

New:

- Full resolution MetOp AVHRR
- SLSTR
- Passive Microwave SST from AMSR-E and AMSR2





SST-CCI Climate Data Record v3



- Includes products at L2P, L3U, L3C, and L4
- SST_{skin} at satellite overpass; SST_{20cm} at 10:30 local time
- Multi-sensor L4 Analysis generated using Met Office OSTIA system





Product Levels





SST is provided at four "product levels":

- **L2P**: data on the Level 1 grid i.e. satellite swath projection
- **L3U**: (uncollated) Level 2 data remapped to global latitude / longitude grid
- **L3C**: (collated) single-sensor observations for a fixed period (daily)
- **L4**: multi-sensor observations blended to a global gap-free product





SST can refer to anything between the interface and ~ 10 m, which varies due to heat flux through the surface.

- SST_{int} is a hypothetical temperature at the exact air-sea interface.
- SST_{skin} the skin temperature measured by an infrared radiometer, corresponds to a depth of ~10-20 µm. This is typically ~0.2 K cooler than in situ measurements (depending on wind speed).
- **SST**_{subskin} the sub-skin temperature. For practical purposes the sub skin can be approximated as the temperature observed by a microwave radiometer.
- **SST_{depth}** temperature measured at any depth below the surface (e.g. SST_{0.2m}), used for the majority of *in situ* measurements (e.g. drifting buoys, ships etc.)



Diurnal Variability



-0.017

24

3-7 m s⁻¹

- SST varies through the day as it is warmed by the sun, and cools at night
 - Typical diurnal cycle is 0.1 0.5 K
 - Can be over 5 K in extreme cases • (low wind, strong sun)
- Satellites observe at various local times of day
- Some satellites are in drifting orbits
- Climate Data Record needs to use standard time of day to avoid aliasing diurnal cycle
- SST CCI uses 10:30 or 22:30 local time •
- Diurnal anomaly is closest to zero, SST is good • approximation for daily average SST



90°S-90°N

0.3

0.2

0.1

0.0

0–3 m s⁻¹

0.3

0.2

0.1

0.0

-0.03

Morak-Bozzo et al. 20160, Geosci. Data J., doi: <u>10.1002/qdj3.35</u>



Dual View Reference Sensors



ATSR

- Unchanged since version 2.1
- Bayesian Cloud detection
- Dual-view coefficient retrieval
 - Based on radiative transfer modelling (LBLRTM)
 - Aerosol robust
 - Fully independent from *in situ*





0.75

-1.00 -0.75 -0.50 -0.25 0.00 0.25 0.50 0.75 1.00 Satellite - in situ / K

AATSR

Merchant et al. 2019, Sci Data, doi:<u>10.1038/s41597-019-0236-x</u>

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Dual View Reference Sensors



SLSTR

- Same fundamental methods as ATSR (Bayesian cloud + dual-view coefficients)
- More complex viewing geometry, wider asymmetric nadir swath
 - CDR processing limited to dual-view overlap
- Two resolutions
 - 500m solar bands (S1 S6)
 - 1 km thermal infrared (S7 S9)
- Level 1b products are presented on a regular grid aligned with sub-satellite track
- Centre of "observation" can be up to ½ pixel from nominal location on grid



SLSTR Regridding



- Centre of "observation" can be up to 1/2 pixel from nominal location on grid
- Cannot use simple 2x2 averaging to map Vis/NIR to TIR channels
 - Misalignment of Vis/NIR will cause cloud detection errors

Coastal example were alignment of TIR scan and nominal grid results in saw tooth edge as "best" IR pixel alternates $+\frac{1}{2}$ and $-\frac{1}{2}$ offset



Bulgin et al. 2023, RSE, doi: 10.1016/j.rse.2023.113531

SLSTR Regridding



- Need to collocate Vis/NIR channels with actual location of 1 km TIR pixels
 - L1b includes both cartesian and geodetic coordinates for every pixel
 - Use k-nearest neighbors to regrid Vis/NIR to TIR pixel locations
 - Include orphan pixels
 - Exclude cosmetic fill



Bulgin et al. 2023, RSE, doi: 10.1016/j.rse.2023.113531

SLSTR Performance



Comparable to ATSR2 / AATSR









-1.00 -0.75 -0.50 -0.25 0.00 0.25 0.50 0.75 1.00 Satellite - in situ / K

	Day Bias	Day RSD	Night Bias	Night RSD
ATSR-2	-0.00	0.28	+0.02	0.24
AATSR	+0.01	0.21	+0.01	0.18
SLSTR-A	+0.02	0.25	+0.00	0.19
SLSTR-B	-0.03	0.24	-0.01	0.19



Single-view AVHRR sensor



AVHRR

- Bayesian Cloud Detection
- Bias-aware Optimal Estimation (OE)
 - Basic OE assumes *a priori* and forward model are zero mean bias and error covariances are known
 - BAOE estimates biases and covariances using a reference dataset

Forward model

• RTTOV 12.3

Improved prior

- CDRv2.1 for SST
- CAMS aerosol including dust

Bias-aware OE

- NOAA AVHRR *in situ*
- MetOp AVHRR AATSR + SLSTR



MetOp AVHRR



- Most AVHRR data are "GAC" resolution
 - "Global Area Coverage"
 - Approximately 4 km size at nadir



GAC pixels (blue) are average of 4 full resolution pixels. White pixels are unused in GAC data

- CDRv2 used MetOp AVHRR at GAC resolution
- CDRv3 uses MetOp AVHRR at full resolution
 - 15 times as many pixels at Level 1 and 2
 - Improves coverage at Level 3

GAC Resolution



Full Resolution



AVHRR: Reduced desert-dust biases



- CDR v2 AVHRR data was affected by cold-biases due to desert-dust aerosol
 - Strong seasonal cycle with biases in Atlantic
 Ocean and Arabian Sea
 - Previous retrieval assumed "clear-sky" with no aerosol present
- CDR v3 adds CAMS aerosol data to prior
 - Includes dust component
 - 2003 2021: CAMS reanalysis
 - Otherwise: CAMS Climatology (Bozzo et al.)
 - Greatly reduces dust biases in AVHRR SST data

Right: NOAA-19 AVHRR daytime minus drifter SST

Bozzo et al. 2020, Geosci. Model Dev., doi: 10.5194/gmd-13-1007-2020

CDR 2.1



CDR 3.0





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AVHRR/1 instruments



- AVHRR/1 instruments had four channels: 0.6, 0.8, 3.8, 11 μm
 - Solar signal affects SWIR, so two channel retrieval only possible at night
- AVHRR/1 used on NOAA-6, -8, and -10 platforms
 - Only sensor available before August 1981

 Not processing TIROS-N in CDRv3

Right: Satellite equator crossing times AVHRR/1 instruments were used for the AM orbit until September 1991 Grey = data not used in CDRv3







- CDRv2 was affected by AVHRR processing failures in 1980s
 - Due to QC checks falsely flagging data received via Wallops Island
 - Resulted in some intermittent coverage gaps during 1980s



AVHRR11_G from 1989-06-20

Top: CDR v2 orbits from WI are missing



CDR 3.0 Day



CDR 3.0 Night



NOAA AVHRR Performance





Metop AVHRR Performance





- Cold bias seen in Arctic SST 2012 2015
- Corresponds to dual-view data gap
- But also seen in unrelated non-CCI products
 - e.g. ACSPO MODIS and VIIRS
- Required further investigation, may indicate a problem with *in situ* measurements





Quality Level (IR Sensors)



- Each pixel is assigned a quality level
- Based on cloud mask (probability of clear), retrieval sensitivity, or goodness-offit test (chi-square)
- QL 4 and 5 recommended or climate applications
- QL 2 and 3 usable for qualitative applications

Level	Meaning	P(clr)	Sens.	Chi ²	Other
0	No data	<0			No data; land pixel
1	Bad data	<0.5	<0.0	>3	SST < 271.15; ice detected, NWP missing
2	Worst quality	<0.8	<0.1	>2	Limb pixel ($\theta_{sat} > 60$)
3	Low quality	<0.9	<0.2	>1	Twilight (87.5 < θ_{sol} <92.5
4	Acceptable				ATSR: aerosol detected AVHRR: solar contamination detected
5	Best quality				

GHRSST Science Team, 2012, Zenodo, doi: 10.5281/zenodo.4700466



Microwave: AMSR



AMSR

- Microwave products were experimental in Phase 2, now included in CDR v3
 - Not affected by cloud, aerosol, water vapour distribution etc.
 - Larger footprint (40 70 km)
 - Limited by proximity to land, sea-ice, RFI, and precipitating cloud
- Retrieval is a two-step linear regression to *in situ*

Sensor	QL	Mean / K	Std. / K
AMSR-E	3	+0.02	0.64
	4	-0.01	0.51
	5	-0.03	0.37
AMSR2	3	+0.02	0.64
	4	+0.01	0.52
	5	-0.00	0.35

Alerskans et al. 2020, RSE, doi: 10.1016/j.rse.2019.111485





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- Retrieval is a two-step linear regression to in situ
- QL is based on retrieval uncertainty so QL 5 limited to tropics

Sensor	QL	Mean / K	Std. / K
AMSR-E	3	+0.02	0.64
	4	-0.01	0.51
	5	-0.03	0.37
AMSR2	3	+0.02	0.64
	4	+0.01	0.52
	5	-0.00	0.35

Alerskans et al. 2020, RSE, doi: 10.1016/j.rse.2019.111485



Single-Sensor Data Density







Level 4 Analysis



- Climate configuration of Met Office OSTIA
 - Only uses SST-CCI L2/3 SST inputs no in situ
 - Sea-ice from EUMETSAT OSI-SAF: OSI-450 and OSI-430-b
 - Global Sea Ice Concentration CDR (and ICDR) release 2
 - Analysis is daily-average SST_{20cm}





Validation against in situ



- SST CCI Independent Reference Data Set (SIRDS)
 - Based on Met Office Hadley Centre Integrated Ocean Dataset (HadIOD)
 - <u>https://www.metoffice.gov.uk/hadobs/hadiod/sirds.html</u>
 - Includes: drifters, gtmba, moorings, ships, argo, bottle, ctd, mbt, xbt, ...
- Variable coverage over CDR period
- Ships provide best coverage in 1980s, but highest uncertainty – typically larger than satellite uncertainty
- Drifters provide majority of obs. since early 2000s, but very limited spatial coverage in 1980s
- Main validation results use:
 - All non-ship *in situ* up to 1995
 - Drifters-only from 1995 onwards



Atkinson et al. 2014, J. Geophys. Res. Oceans, doi: <u>10.1002/2014JC010053</u>



Time series of IR validation against in situ



Summary of IR validation against in situ



	D	ау	Nig	Night	
	Median	RSD	Median	RSD	
NOAA-06			+0.02	0.55	
NOAA-07	+0.00	0.53	+0.07	0.53	
NOAA-08			+0.02	0.57	
NOAA-09	+0.02	0.49	+0.02	0.51	
NOAA-10			-0.04	0.52	
NOAA-11	+0.07	0.43	+0.05	0.41	
NOAA-12	+0.02	0.40	-0.00	0.41	
NOAA-14	+0.04	0.37	+0.02	0.38	
NOAA-15	+0.03	0.32	+0.03	0.34	
NOAA-16	+0.05	0.30	-0.03	0.29	
NOAA-17	+0.07	0.25	+0.06	0.26	
NOAA-18	+0.03	0.28	-0.02	0.27	
NOAA-19	+0.05	0.28	-0.03	0.25	

Reference in situ includes all non-ship data up to NOAA-12

Drifters-only used for NOAA-14 onwards

Summary of IR validation against in situ



	Da	ay	Night	
	Median	RSD	Median	RSD
MetOp-A	-0.01	0.25	-0.01	0.24
MetOp-B	+0.01	0.25	+0.02	0.24
ATSR-1	+0.04	0.45	+0.01	0.45
ATSR-1 (d3)			+0.00	0.26
ATSR-2	-0.00	0.28	+0.02	0.21
AATSR	+0.01	0.21	+0.01	0.18
SLSTR-A	+0.02	0.25	+0.00	0.19
SLSTR-B	-0.03	0.24	-0.01	0.19



Uncertainties



- SST CCI products also include estimates of retrieval uncertainty
- Broken down into components for single-sensor Level 2 / 3 products:
 - Random uncertainty due to effects which are uncorrelated from pixel to pixel (e.g. instrument noise)
 - Correlated uncertainty due to effects which are assumed to be correlated over scales ~100 km / ~1 day (e.g. atmospheric effects)
 - **Adjustment** uncertainty in the time and depth adjustment





- Uncertainties can be validated using *in situ* data
- **Right**: discrepancy (satellite *in situ*) against estimated uncertainty
- Grey area shows robust standard deviation (RSD) of discrepancy
- Blue line shows expected dependency from assumed *in situ* uncertainty (0.2 K for drifters)
- Green violin plot shows distribution of data





- Dual-view (ATSR-2 onwards) uncertainties are generally well estimated
- ATSR-1 uncertainties are slightly underestimated
- Largest SLSTR uncertainties are underestimated
- Most SST values have low estimated uncertainties
 - Day $\lesssim 0.2 \text{ K}$
 - Night $\lesssim 0.1 \text{ K}$



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- Single-view nighttime uncertainties are generally well estimated
- Daytime uncertainty estimates are not skillful





- Level 4 analysis uncertainty are slightly over-estimated
- Maybe partly related to *in situ* data

 reference data had a median
 reported uncertainty of 0.39 K
- Majority of data have estimated uncertainty < 0.5 K
- Data are more uncertain in coastal regions





Interim-CDR



- Ongoing extension of SST-CCI CDR produced using the same software
 - Uses ECMWF ERA5-T as prior rather than ERA5 (CDR)
 - 2-3 weeks behind present
- With version 3 both CDR and ICDR will be accessed as a single dataset via CEDA
- 2022 funded by Copernicus Climate Change Service (C3S)
- 2023 onwards funded by:
 - UK Earth Observation Climate Information Service (EOCIS) Level 2/3 production (Reading)
 - Marine Climate Advisory Service (MCAS) Level 4 production (Met Office)



Interim-CDR







Surftemp.net



- Steady stream of requests from users with less compute capability to deal with full SST CCI archive data on CEDA
- For flexible low-resolution and extraction requests: <u>https://surftemp.net/</u>
- Region, time period and resolution requested are ordered, and users download from a link after creation
- Regridded uncertainties are also estimated
- Made under NCEO funding
- 77 subscribed users plus many anonymous

Sea Surface Temperature Data

The data available here is made available by the <u>Surface Temperature Group at the University of Reading, UK</u>. To obtain the data upon which these services are based, see <u>data used by this service</u>.

Available services

Re-gridding Service

Obtain L4 sea and ocean surface temperature datasets in your chosen spatial and temporal resolution



Time-series Service

Obtain L4 sea and ocean timeseries for a particular bounding box

Region Service

Obtain L4 sea and ocean data at 0.05 degree resolution for a particular bounding box



Subscription

Subscribe to or unsubscribe from e-mail notifications of new data or features

For any questions, suggestions or issues with using this service, please contact n.f.mccarroll@reading.ac.uk.







Intercomparison: Recent Warming



CMC

- ICOADS (GTS from 2007) Ship + Buoy
- NAVO AVHRR
- REMSS: TMI, Windsat, AMSRE, AMSR2
- OSPO VIIRS
- EUR ATSR

OSTIA Reprocessing 2.0

- HadIOD Buoy
- ESA CCI v2.1: AVHRR, ATSR, SLSTR
- REMSS: TMI, GMI, AMSRE, AMSR2
- OSI-SAF: GOES-13, GOES-16, SEVIRI

DOISST

- ICOADS (GTS for 2007-2016) Ship + Buoy
- Argo from 2016 onwards
- 1981-2006: AVHRR Pathfinder
- 2007-2021: NAVO AVHRR
- 2021-onwards ACSPO MetOp-B + VIIRS

OSTIA 2.0 analysis combines ESA CCI v2.1 L2/3 with other satellite and in situ to produce a foundation SST

• not the same as CCI Analysis SST 2.1

DOISST is only product to include Argo

Intercomparison: Recent Warming



ESA CCI.v3.0 ____ 2021 _____ 2022 - 2023 --- 1982-2011 mean --- ± 20 21.0 21.0 20. 19.5 -19.5 -Jan Mav lun Aug Oct Dec lan OSTIA 2.0 (NRT from 2022) 21. 2021 _____2022 - 2023 --- 1982-2011 mean --- ± 20 21.0 21.0 20.0 19.5 Jun Jul Aug Oct Dec Jan Sen Day of Year



Intercomparison



CMC

- ~0.15 K trend from 1991 to 2000
- match within 0.05 K from ~2002

DOISST

- ~0.1 K cooler in 1980/90
- 0.1 K step change in 2020
 OSTIA
- Dual-view gap 2012-2017
- Includes NRT from 2022



Mean Global SST (ESA CCI v3.0)





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SST CCI Oct 2023 | Reading | Slide 40







- 42-year CDR from 1980 to end-2021
 - Adds AVHRR/1, Passive Microwave, full-resolution MetOp, and SLSTR
 - New bias-aware OE retrieval and reduced desert-dust related biases
- Interim-CDR to provide ongoing extension at 2-3 weeks latency
 - 2022: C3S
 - 2023 onwards: UK funding EOCIS / MCAS
- Public data release will be late 2023 via the CCI Open Data Portal
 - <u>https://climate.esa.int/en/odp/</u>
- Regional and re-gridded data products:
 - <u>https://surftemp.net/</u>