Algorithm Theoretical Basis Document for Geostationary Satellite Sea Surface Temperature

OSI-206-a; OSI-207-b; OSI-IO-SST

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Documentation change record

Version	Date	Authors	Description
0.1	11/3/2019	MF	Initial submitted version - This document supersedes the ATBD for the GOES-16 SST and contains also the information relative to Meteosat SST.
1.0	29/3/2019	MF	The main differences in the updated processing of SST are: • gaussian kernel smoothing of the (T10.8-T12.0) term of the SST algorithm (see equation 3 of the ATBD) instead of box average. • the brightness temperature adjustment (section 3.2.2 in the ATBD), for the SST algorithm correction, now relies on 3 days of most recent data, whereas it is 20 days in the current processing (with decreasing weight the further we are from processing time). It was identified as a simplification of the processing rather than an actual improvement of the quality of the final product. Although we have checked that it did not alter its quality. Tests were performed for the reprocessing of SEVIRI datarecord (OSI-250). • the brightness temperature adjustment is also using Gaussian kernel smoothing instead of box average.
1.1	8/11/2019	MF	Editorial correction: Hourly product definition (section 4).
1.2	5/7/2022	MF	Switch to Meteosat-9 over Indian Ocean.
1.3	15/3/2023	MF	Meteosat-10 replace Meteosat-11 in 0° position on the 21th of March 2023.
1.4	10/10/2023	MF	SST coefficients adjustment for Meteosat-10.

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1 Introduction

The EUMETSAT Satellite Application Facilities (SAFs) are dedicated centres of excellence for processing satellite data. They form an integral part of the distributed EUMETSAT Application Ground Segment. The Ocean and Sea Ice SAF, led by Météo-France (MF), has the responsibility of developing, validating and distributing near real time products of Sea Surface Temperature (SST), radiative fluxes, wind and Sea Ice parameters for a variety of platforms/sensors.

As part of the Fourth Continuous Development and Operations Phase (CDOP4 2022-2027) OSI SAF (more specifically MF) has committed to provide user community with operational product of Sea Surface Temperature (SST) and Radiative Fluxes from the American Geostationary Operational Environment Satellite (GOES) in East position, the Meteosat Second Generation (MSG) in position 0°. OSI SAF is also providing SST and radiative fluxes for MSG Indian Ocean on a best effort basis. Currently OSI SAF is processing data from:

- GOES-16 which was launch on the 19th of November 2017 and was declared operational in East position (75.2°W) on the 18th of December 2017.
- Meteosat-10 which has operationally replaced Meteosat-11 in 0° position on the 21th of March 2023. Before this date it was Meteosat-11 which had been launched on the 15th of July 2015 and had operationally replaced Meteosat-10 on the 21th of February 2018.
- Meteosat-9 which has operationally replaced Meteosat-8 over Indian Ocean in 45.5°E on the 23rd of June 2022.

OSI SAF SST products are designed to answer the need of the scientific and meteorological communities in several domains such as regional NWP, oceanography and operational oceanography or fisheries.

1.1 Reference documents

Ref	Title	Code
[RD.1]	Scientific Validation Report for the Geostationary Satellite Sea Surface Temperature	SAF/OSI/CDOP3/MF /SCI/RP/371 Documentation on OSI SAF web site
[RD.2]	Algorithm Theoretical Basis Document for the Cloud Product Processors of the NWC/GEO, version 10d	NWC/CDOP2/GEO/MFL /SCI/ATBD/Cloud Documentation on NWC SAF web site

1.2 Applicable documents

Ref	Title	Code
[AD.1]	Product Requirement Document	Project Documentation on OSI SAF web site

1.3 Purpose and scope of the document

This document describes the algorithms and methods implemented in the current processing chain for geostationary satellites SST production from GOES-16/ABI (product OSI-207-b), Meteosat-10 (product OSI-206-a) and Meteosat-9 (product OSI-IO-SST) with the characteristics summarized in table 1. It also gives a brief overview of the datasets to used in the processing.

Table 1: Geostationary products summary.

Product ID	Satel-lite/instrument	Spatial coverage	Spatial sampling	Frequency	Reference
OSI-207-b	GOES-16/ABI	60°N to 60°S 135°W – 15°W	0.05° Lat-Lon	hourly	[AD.1]
OSI-206-a	Meteosat-10 /SEVIRI	60°N to 60°S 60°W – 60°E	0.05° Lat-Lon	hourly	[AD.1]
OSI-IO-SST	Meteosat-09 /SEVIRI	60°N to 60°S 14.5°W – 105.5°E	0.05° Lat-Lon	hourly	

This document is complemented by a scientific validation report (SVR) and a product user manual (PUM) also available on the OSI SAF website.

1.4 Scientific background

SST retrieval from infrared (IR) radiometer measurements classically uses multichannel algorithms (e.g. **?**). More recent developments have improved retrieval through the usage of atmospheric profiles of temperature and water vapour provided by Numerical Weather Prediction (NWP) models in order to correct for regional and seasonal biases. OSI SAF (at MF) has long term experience in using the algorithm correction method in the newer processing chains for MSG/SEVIRI and Metop/AVHRR. This method developed by **?** uses NWP output together with a guess SST (analysis) and a radiative transfer model to simulated Brightness Temperatures (BT) for each pixels. It then uses this information to compute a so-called simulated SST using the multichannel algorithm to be corrected for regional and seasonal biases. Under some conditions and hypothesis, the difference between guess SST and simulated SST is the algorithm error with respect to specific atmospheric conditions.

Another similar approach have been developed by **?** and further enhanced in **?**. It is also based on NWP data and simulation of BTs. An inversion method is used to explain the differences between simulated and observed BTs in terms of SST correction.

Both methods aforementioned requires a step of adjustment of the simulated BTs. This step is designed to ensure that simulated BTs are not biased by uncertainties in the radiative transfer model used and its inputs.

As of today there is no real consensus about the best method. Historically OSI SAF is using the multichannel algorithm and the algorithm correction method aforementioned. Operational processing chains for MSG/SEVIRI and Metop/AVHRR using this method have shown good and consistent results. For this reason the same approach is chosen for GOES-16/ABI SST processing.

SST products quality are assessed with respect to the product requirements [AD.1] and the validation results obtained for operational processing are presented in [RD.1].

1.5 Characteristics of MSG/SEVIRI instrument

MSG payload include the SEVIRI instrument. The SEVIRI radiometer is a multi-channel passive imaging radiometer operating in twelve channels (Figure 1). The full disk is scanned with a repeat cycle of 15 minutes.

Channel No.	Spectral Band (µm)	Characteristics of Spectral Band (µm)			Main observational application
		λ_{cen}	λ_{min}	λ_{max}	
1	VIS0.6	0.635	0.56	0.71	Surface, clouds, wind fields
2	VIS0.8	0.81	0.74	0.88	Surface, clouds, wind fields
3	NIR1.6	1.64	1.50	1.78	Surface, cloud phase
4	IR3.9	3.90	3.48	4.36	Surface, clouds, wind fields
5	WV6.2	6.25	5.35	7.15	Water vapor, high level clouds, atmospheric instability
6	WV7.3	7.35	6.85	7.85	Water vapor, atmospheric instability
7	IR8.7	8.70	8.30	9.1	Surface, clouds, atmospheric instability
8	IR9.7	9.66	9.38	9.94	Ozone
9	IR10.8	10.80	9.80	11.80	Surface, clouds, wind fields, atmospheric instability
10	IR12.0	12.00	11.00	13.00	Surface, clouds, atmospheric instability
11	IR13.4	13.40	12.40	14.40	Cirrus cloud height, atmospheric instability
12	HRV	Broadband (about 0.4 – 1.1 µm)			Surface, clouds

Figure 1: Spectral channel characteristics of SEVIRI in terms of central, minimum and maximum wavelength of the channels and the main application areas of each channel http://oiswww.eumetsat.org/WEBOPS/msg_interpretation/msg_channels.php

1.6 Characteristics of GOES/ABI instrument

GOES-16 payload include the Advanced Baseline Imager (ABI) which is primarily designed to retrieve cloud parameters, horizontal winds and integrated water vapour. Its infrared channels also enable retrieval of SST.

ABI is a multi-channel passive imaging radiometer operating in sixteen channels: two in the visible region of the spectrum, four in the near infrared and ten in the infrared (Figure 2). The spatial resolution at the satellite sub-point is 2 km for infrared channels (of interest for SST retrieval). The full disk is scanned with a basic repeat cycle of 15 minutes [AD.2].

Table I. Summary of the wavelengths, resolution, and sample use and heritage instrument(s) of the ABI bands. The minimum and maximum wavelength range represent the full width at half maximum (FWHM or 50%) points. [The Instantaneous Geometric Field Of View (IGFOV).]

Future GOES imager (ABI) band	Wavelength range (μm)	Central wavelength (μm)	Nominal subsatellite IGFOV (km)	Sample use	Heritage instrument(s)
1	0.45–0.49	0.47	1	Daytime aerosol over land, coastal water mapping	MODIS
2	0.59–0.69	0.64	0.5	Daytime clouds fog, insolation, winds	Current GOES imager/ sounder
3	0.846–0.885	0.865	1	Daytime vegetation/burn scar and aerosol over water, winds	VIIRS, spectrally modified AVHRR
4	1.371–1.386	1.378	2	Daytime cirrus cloud	VIIRS, MODIS
5	1.58–1.64	1.61	1	Daytime cloud-top phase and particle size, snow	VIIRS, spectrally modified AVHRR
6	2.225–2.275	2.25	2	Daytime land/cloud properties, particle size, vegetation, snow	VIIRS, similar to MODIS
7	3.80–4.00	3.90	2	Surface and cloud, fog at night, fire, winds	Current GOES imager
8	5.77–6.6	6.19	2	High-level atmospheric water vapor, winds, rainfall	Current GOES imager
9	6.75–7.15	6.95	2	Midlevel atmospheric water vapor, winds, rainfall	Current GOES sounder
10	7.24–7.44	7.34	2	Lower-level water vapor, winds, and SO_2	Spectrally modified current GOES sounder
11	8.3–8.7	8.5	2	Total water for stability, cloud phase, dust, SO_2 rainfall	MAS
12	9.42–9.8	9.61	2	Total ozone, turbulence, and winds	Spectrally modified current sounder
13	10.1–10.6	10.35	2	Surface and cloud	MAS
14	10.8–11.6	11.2	2	Imagery, SST, clouds, rainfall	Current GOES sounder
15	11.8–12.8	12.3	2	Total water, ash, and SST	Current GOES sounder
16	13.0–13.6	13.3	2	Air temperature, cloud heights and amounts	Current GOES sounder/ *GOES-12+* imager

Source: Schmit, T.J., Gunshor, M.M., Menzel, W.P., Gurka, J.J., Li, J., Bachmeier, A.S., 2005, Introducing the Next-Generation Advanced Baseline Imager on GOES-R, Bulletin of the American Meteorological Society, v. 86, p. 1079-1096.

Figure 2: Channels of ABI instrument `https://www.goes-r.gov/spacesegment/ABI-tech-summary.html`

1.7 Acronyms and definitions

The term workfile is used to designate intermediary files produced by the processing chain. Workfiles contains most of the intermediate variables of the processing.

ABI	Advanced Baseline Imager
AOD	Aerosol Optical Depth
AVHRR	Advanced Very High Resolution Radiometer
BT	Brightness Temperature
CSPP	Community Satellite Processing Package
ECMWF	European Centre for Medium-range Weather Forecasts

GDS	GHRSST Data Specification
GHRSST	Group for High Resolution SST
GTS	Global Telecommunication System
GOES	Geostationary Operational Environment Satellite
IR	Infrared
MF	Météo-France
MDS	Matchup DataSet
MSG	Meteosat Second Generation
Metop	Meteorological Operational
NAAPS	Navy Aerosol Analysis and Prediction System
NWP	Numerical Weather Prediction
NWP SAF	Numerical Weather Prediction Satellite Application Facility
OSI SAF	Ocean and Sea Ice Satellite Application Facility
OSTIA	Operational Sea Surface Temperature and Sea Ice Analysis
PUM	Product User Manual
QL	Quality Level
RTM	Radiative Transfer Model
RTTOV	Radiative Transfer for TOVS
SAF	Satellite Application Facility
SDI	Saharan Dust Index
SEVIRI	Spinning Enhanced Visible and InfraRed Imager
SSES	Sensor Specific Error Statistics
SST	Sea Surface Temperature
SVR	Scientific Validation Report

2 Overview of the processing

In this section a brief overview of the input datasets used and the main steps of the processing are given.

2.1 The main steps of the processing

The processing can be divided into a few main steps:

1. *Simulations of BT*: A Radiative Transfer Model (RTM) is used for computing simulated BTs for every clear sky sea and lake pixels and for each IR channel used for SST retrieval and every three hours. Currently we use Radiative Transfer for TOVS (RTTOV, **?**) version 12. Inputs to this RTM include forecasts of atmospheric profiles of water vapour from a ECMWF model and a guess SST (OSTIA analysis).

2. *BTs adjustment*: This step is of primary importance because it is designed to ensure that the simulated BTs are not biased by uncertainties in the RTM and its input data. See section 3.2.2 for details.

3. *Control of the mask*: This step is designed to detect possible problems such as remaining cloud contamination. It consists in a series of tests which are contributing to the Quality Level (QL) assignment (see section 2.3). These tests are performed at various stage of the processing depending on the tested values.

4. *SST retrieval*: A classical non-linear SST algorithm is used to provide a first estimate of the SST (see section 3.1). It is used in particular in the control of the mask.

5. *SST algorithm corrections*: Le Borgne et al. (2011) algorithm correction scheme is used (section 3.3) to reduce regional and seasonal biases.

6. Computation of *Single Sensor Error Statistics (SSES)*

7. Production of *hourly synthesis* and *GHRSST compliant L3C product* from 15 minutes workfiles.

These steps are not applied in a sequential order, in fact they are not even performed with the same time step. Simulation of BTs are performed every three hours as NWP forecasts are produced on a three-hourly basis. BT adjustment field is computed on daily basis, they are used to elaborate the algorithm correction fields every three hours. Hourly synthesis are computed at round hours. The hourly synthesis for H includes SST computed at all slots in the interval $[H-30, H+15]$. However, please note that the production of SST for the slots in the interval $[H-30, H+15]$ requires the reception of the slots within the interval $[H-60, H+45]$, see section 2.3 for clarification (table 2, SST temporal variability).

2.2 Data

The data used in the processing are listed below. They are described in their version available at the time of the writing of this document. It is likely that this list will evolve in the future to make use of the best dataset available.

2.2.1 MSG/SEVIRI and GOES/ABI level 1 data

Input data for the processing chain mostly consist in brightness temperature at wavelength used for SST retrieval and Saharan Dust Index computation (only for SEVIRI). These are computed at MF using the CSPP Geo software (Community Satellite Processing Package for Geostationary Data:
http://cimss.ssec.wisc.edu/csppgeo/)

2.2.2 Dynamic ancillary data

- 3-hourly atmospheric temperature and humidity profiles (plus a few surface fields) from NWP model. Nowadays European Centre for Medium-Range Weather Forecasts (ECMWF) data are used in SST operational chains.
- An SST analysis is needed for simulations of BTs. Nowadays, this analysis is the OSTIA SST daily analysis (**?**).
- The cloud mask originates from the Cloud Product Processor of the NWC SAF which is run at MF [RD.2].

2.2.3 Auxillary datasets

These are the static datasets such as climatologies. They include the data being used nowadays by OSI SAF for operational processing.

- Foundation SST climatology. Currently a climatology based on OSTIA daily SST re-analyses (1985-2007) is used (**?**).
- SST front climatology developed by the University of Rhodes Island.
- Land/Sea/Lake mask: ARC-Lake

2.3 Quality level and test indicators: control of the cloud mask

The control of the cloud mask consists in a series of tests designed to identify pixels contaminated by undetected clouds or atmospheric dust aerosols for instance. We use the concept of indicator to quantify, in an empirical way, the risk of having an error in the SST retrieval because of uncertainties in algorithms or ancillary variables. For each test, the tested quantity (tested_value) is compared to a limit value (limit_value) and to a critical value (critical_value). Outside this range there is either no problem or the risk of error is too high. The core definition of the test indicator is given below, however many other factors can influence each indicators (for example availability of ancillary data used in the definition of the indicator) that are not detailed here:

$$\text{test\_indicator} = 100(\text{tested\_value} - \text{limit\_value})/(\text{critical\_value} - \text{limit\_value}) \quad (1)$$

There is a range of test_value, for example: the difference between the climatological SST and the retrieved SST, the SDI, the distance to cloud, etc. [limit_value, critical_value] define a range of the test_value below and above which the test_indicator is 0 and 100 respectively.

The formulation above has the advantage of homogenising all the indicators on a unique scale:

- 0: no problem
- $]0, 100[$: potential problem

- 100: critical problem

There are two types of indicators: (i) the common indicators, independent of the SST retrieved and the algorithm used, they are generic to the whole processing. They include the dust indicator, the distance to cloud indicator and the ice indicator. (ii) The specific indicators, based on the value of the SST retrieved in comparison to climatologies of SST and SST gradients (the SST value indicator and the SST gradient indicator). At the end of the processing all these indicators are combined into one single indicator by means of a weighted average: this is the SST mask indicator.

Two other indicators are defined that do not enter in the SST mask indicator, but are considered for determining the quality level: the indicator reflecting the uncertainties of the SST algorithm with respect to the satellite zenith angle (algorithm indicator), and the indicator about the confidence we have in the correction term (the SST correction indicator).

A brief description of the tests is given in table 2:

Table 2: List of indicators contributing to the quality level

Test	**Description/purpose**
SST value	This test aims at attributing a lower quality level to SST values too different from climatology. The local value of estimated SST is compared to a climatology of SST, the larger the difference between estimated SST and SST climatology, the higher the indicator.
SST spatial variability	The main objective of this test is to attribute a lower quality level to pixels in areas where the gradients are unrealistically large due to the presence of undetected cloud cover in most cases. The local value of the SST gradient is compared to a climatology of maximum gradient.
SST temporal variability	The main objective of this test is to attribute a lower quality level to pixels displaying a fast changing SST suggesting that some cloud contamination is occurring. Practically, the BT in one IR channel at a given time T is compared to the BT before (at $T - 30$ minutes) and after (at $T + 30$ minutes).
Aerosol dust	This test influences the quality level of pixels contaminated by Saharan dusts. It is directly related to the Saharan Dust Index when available (for SEVIRI only) or the Aerosol Optical Depth in other cases (see section 3.4).
Distance to cloud	Pixels in the immediate vicinity of clouds are likely to be partly covered by cloud or affected by transparent undetected clouds.
Sea ice	The purpose of this test is to degrade the quality of pixels suspected to contain ice.
Satellite zenith angle	The test takes into account the fact that high satellite zenith angle is likely to lead to higher uncertainty because of higher atmospheric optical depth. The resulting indicator is directly linked to the satellite zenith angle.
SST correction	This test is based on the assumption that high SST corrections are associated with high uncertainties. It is directly linked to the value of the SST correction. It is only applied in the algorithm correction method.

Quality levels are designed to help users to filter out data that are not sufficiently good for their applications. It is essential to adopt the recommendation of the GHRSST formalised through the GDS v2 document. For infrared derived SST six quality levels are defined. 0: unprocessed; 1: cloudy, 2: bad, 3: suspect, 4 acceptable, 5 excellent.

The value of the quality level is determined by examining the values of three indicators: the SST mask indicator (resulting from several sub-indicators as explained above), the algorithm indicator and the SST correction indicator (only in the case of the algorithm correction method, see section 3.3). The poorest indicator will drive the value of the quality level.

3 SST algorithm

In this section we present the “classical” SST algorithm used in the control of the mask, the method for bias correction of SST based on simulation of BTs, and the method envisaged for taking into account atmospheric Saharan dust contamination.

3.1 Non-linear SST algorithm

A classical non-linear SST algorithm will be used to provide a first estimate of the SST. This estimate is used in various steps of the processing, it is referred to as the “classical” and it is:

- used in the calculation of an initial value of some indicators and QL (see section 2.3).
- used in the brightness temperature adjustment step (see section 3.2.2)
- the basis of the algorithm correction method (see section 3.3)

Non-linear algorithm have been used for a long time for retrieving SST from BTs in infrared channels (**??**) measured by a variety of instruments such as AVHRR and SEVIRI. These algorithms have the following generic form:

$$\hat{\mathrm{x}} = a_0 + \mathbf{a}^\top \mathbf{y}_0 \tag{2}$$

where, $\hat{\mathrm{x}}$ is the estimated SST, a_0 is an offset coefficient, $\mathbf{a}$ is a column vector of weighting coefficients and $\mathbf{y}_0$ contains the observed BTs. The coefficients contained in the vector $\mathbf{a}$ are potentially functions of SST climatology and satellite zenith angle.

In the case of MSG/SEVIRI operational processing the algorithm uses two channels and have the following form:

$$\mathrm{SST} = (a + b\,S_\Theta)\,T_{10.8} + (c + d\,S_\Theta + e\,T_{clim})(T_{10.8} - T_{12.0}) + f + g\,S_\Theta \tag{3}$$

where $T_{10.8}$ and $T_{12.0}$ are the observed brightness temperature at the central wavelength of 10.8 and 12.0μm respectively.

In the case of GOES/ABI operational processing the algorithm uses three channels and have the following form:

$$\mathrm{SST} = (a + b\,S_\Theta)\,T_{8.5} + (c + d\,S_\Theta + e\,T_{clim})(T_{10.3} - T_{12.3}) + f + g\,S_\Theta \tag{4}$$

where $T_{8.5}$, $T_{10.3}$ and $T_{12.3}$ are the observed brightness temperature at the central wavelength of 8.5, 10.3 and 12.3μm respectively, $S_\Theta = sec(\Theta) - 1$ and Θ is the satellite zenith angle. T_{clim} is the climatological temperature.

The term $(T_{10.8} - T_{12.0})$ in equation 3 and $(T_{10.3} - T_{12.3})$ in equation 4 is used in this “split-window” algorithms to correct for absorption by water vapour in the atmosphere. However, this term is also particularly sensitive to radiometric noise; it is therefore smoothed over boxes (of a size 9×9 in which the atmosphere is assumed to be homogeneous) by a Gaussian filter, applied to clear/no ice pixels. This classical procedure reduces the noise in the retrieved SST.

The parameters of equation3 and 4 are determined by regression using simulation of BTs computed on a dataset of atmospheric profiles from NWP model using RTTOV radiative transfer model. This step is generally performed before launch as soon as the filter function of the instrument are known to us. A second step consists in adjusting the last two parameters of equation 4 (f and g) using drifting buoys measurements. This step is generally done when enough collocation data (between satellite and drifting buoys) have been collected, typically a few months.

The values of the coefficients are given in table 3. They are unique for day and night time conditions.

Table 3: Coefficients of the non linear split window night-time algorithms for Meteosat-9, Meteosat-10, and for GOES-16 with all temperatures expressed in Celsius.

	a	b	c	d	e	f	g
GOES-16 19/11/2019 to now	1.01021	0.03494	1.20393	0.29217	0.01411	2.17338	1.25504
Meteosat-10 02/10/2023 to now	0.98946	0.0	0.0	1.08181	0.07022	1.66423	0.20510
Meteosat-9 23/06/2022 to now	0.98766	0.00417	0.39558	0.54305	0.05624	1.09287	0.94413

Since the coefficients of the SST algorithm are established using simulations from RTTOV radiative transfer model and de-biased against drifting buoys measurements (at a depth of 20 to 30 cm), the retrieved SST is considered to be the sub-skin SST. One could apply a −0.17°C (**?**) to get the skin SST. However this offset is only a very rough conversion term valid at large scale for wind speed generally exceeding $6\,\mathrm{m/s^{-1}}$.

3.2 Brightness temperature simulation and adjustment

3.2.1 Brightness temperature simulation

Simulation of BTs are performed for each clear-sky sea or lake pixel using RTTOV. Input variable to RTTOV are described in section 2.2 and summarized here:

- A first guess of SST (SST^{guess}, which is a SST analysis such as OSTIA daily analysis).
- Atmospheric temperature and humidity profiles from NWP model.
- Instrument filter functions in the infrared channels.

Simulations are performed at the time step of the input model data which is 3-hourly and for the channels of interest for SST computation.

3.2.2 Brightness temperature simulation adjustment

Before their usage in the algorithm correction or in the optimal estimation, BTs must be adjusted to correct for systematic differences with respect to the observations. These differences can be due to:

- NWP atmospheric profiles uncertainties
- Atmospheric profile sampling
- RTTOV uncertainties
- Filter function and calibration uncertainties

In a synthetic way, we use the difference between simulations and satellite observations (spatially and temporally smoothed out) and interpret the differences as an adjustment term. The description of the BT adjustment method is provided in detailed in **?** for Metop/AVHRR.

The major hypothesis of the BT adjustment is that there is no average bias between the guess SST (used in BTs simulation) and the true SST. It is therefore crucial to properly filter out cases (pixels) where the observed SST cannot be compared with guess SST (for example if there is a diurnal cycle or cloud contamination). Such filtering includes:

- Quality level filtering: only good quality SST retrievals are used (QL $\geq$ 4)
- Atmospheric dust aerosol filtering based on the dust aerosol indicator
- SST filtering: we ensure that “classical SST” and guess SST are close to each other (less than 1K difference)
- Elimination of cases where there is a risk of diurnal warming. Filter based on wind speed at 10 meters, solar zenith angle (Θ_{sol}) and a threshold on the difference between observed and simulated BTs.
- Only night-time pixels are kept except at high latitude where day-time pixels are allowed if the difference between simulated and observed BT at 10.3 μm is smaller than 0.5°C.

Filtered data are averaged temporally and spatially every day at 00h UTC using only slots at 00h UTC $\pm$ 3h on a 3-dimensional low resolution grid ($1 \times 1°$). When computing the BT adjustment, these fields are averaged over 3 days (3 fields) and the result is smoothed out by applying a Gaussian kernel (radius = 5°, $\sigma = 2$). In order to fill in any remaining gaps, successive smoothing are applied with increasing kernel size. One such field is produced for each channel and at 00h UTC every day and used during the following day. Adjustments are then added to BT simulations to produce adjusted BT simulations (3-hourly). This procedure has been elaborated and used for the OSI SAF processing of Meteosat-8 and Meteosat-9 SST data record. Figure 3 shows an example of the adjustment field (right) for GOES-16.

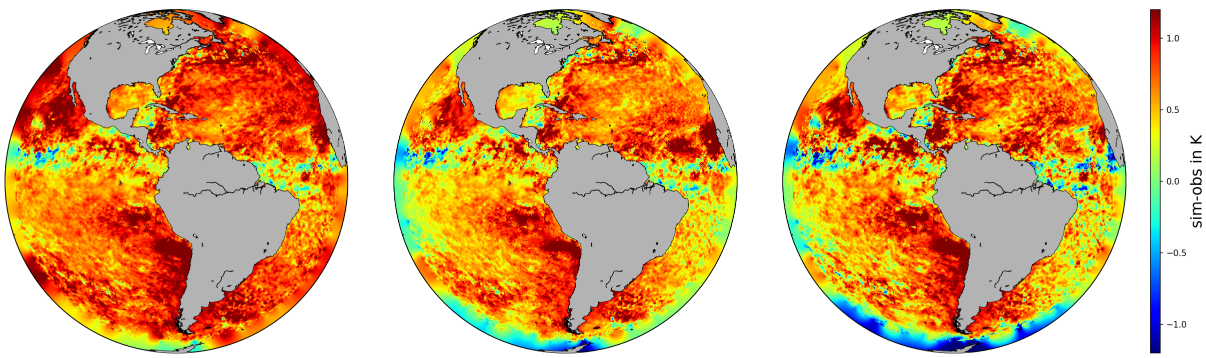

Figure 3: Adjustment field for IR 8.5 (left), 10.3 (middle) and 12.3 (right) of GOES-16/ABI (right): simulated BTs - observed BTs. Date: 6/6/2018 - 0h.

3.3 Corrected SST

The method of algorithm correction was developed by **?**, it is used today in the operational processing of OSI SAF SST products from Metop-B and MSG/SEVIRI. Operational SST delivered in those products is the corrected SST.

A so-called "simulated" SST (SST^{sim}) is computed from simulated BTs adjusted (see section 3.2.2) using the non-linear algorithms described in section 3.1.

The following difference is then computed:

$$\Delta SST = SST^{sim} - SST^{guess} \tag{5}$$

Since the BT simulations used to compute SST^{sim} have been adjusted to correct for uncertainties linked with RTTOV and atmospheric water vapour profiles, ΔSST represent the error due to the algorithm which is unable to cope with all atmospheric conditions.

The corrected SST (SST^{cor}) is then computed as follow:

$$SST^{cor} = SST^{obs} - \Delta SST \tag{6}$$

where SST^{obs} is the "classical" SST as computed by the algorithm presented in section 3.1.

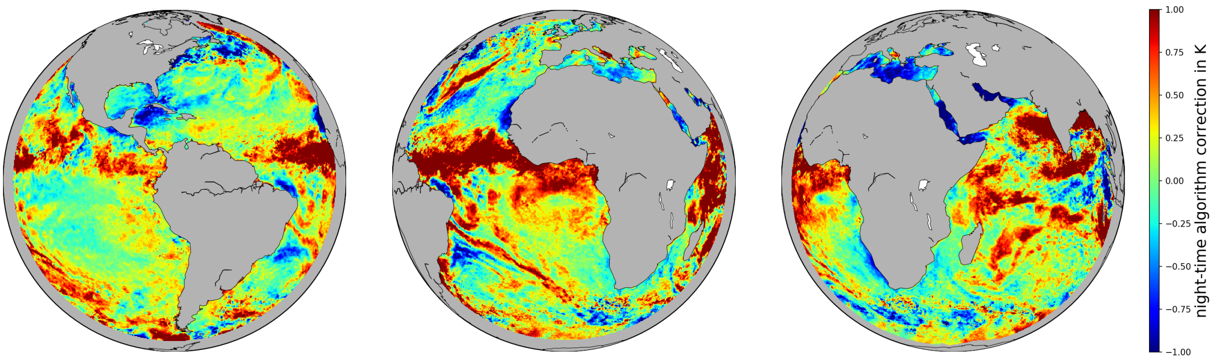

Figure 4: Example of SST algorithm correction field for GOES-16/ABI, Meteosat-11/SEVIRI and Meteosat-8/SEVIRI on the 6th of June 2018.

In practice SST algorithm correction fields are computed at the same time step as the simulations (3-hourly) and the correction is linearly interpolated to each slot time.

3.4 Saharan dust contamination

Saharan dusts in the atmosphere have the effect of attenuating the signal received by the sensor therefore leading to an underestimation of SST. Saharan dusts originate from the Saharan desert and travel westward in the atmosphere in a latitudinal band roughly between O and 30° N in the Atlantic. They can also be present over the Mediterranean sea.

The algorithm described in section 3.1 and the method of correction described in section 3.3 do not take into account Saharan dusts. It is therefore essential to correct for such phenomenon, it is generally performed as a post correction once the SST has been calculated.

The instrument SEVIRI on-board MSG satellites enable the computation of the so-called Saharan Dust Index (**?**) which is computed for night time with equation 7. During day time, because IR 3.9 is contaminated by sun light, another equation is used (equation 8) and its coefficients are determined locally by regression against night time SDI.

$$\mathrm{SDI}_{\mathrm{night}} = S_1(T_{3.9} - T_{8.7}) + S_2(T_{10.8} - T_{12.0}) + S_3 \tag{7}$$

$$\mathrm{SDI}_{\mathrm{day}} = DS_1T_{8.7} + DS_2T_{10.8} + DS_3T_{12.0}DS_4T_{13.4} + DS_5 \tag{8}$$

Unfortunately there is no equivalent for GOES/ABI, the channels being different and not sensitive in the same way to atmospheric dust aerosols. However the nearest SDI produced by the operational MSG processing is used to identify pixels potentially contaminated. Their quality level is then affected through the dust aerosol indicator (see section 2.3). This is only possible for the common area between MSG and GOES-16. For the other pixels (or when SDI information is missing) we rely on NAAPS Aerosol Optical Depth (AOD) to degrade the pixel's quality level.

4 Hourly synthesis

SST is computed for every 15 minutes slot going through the processing chain. The intermediate primary workfiles resulting are to be aggregated into hourly workfiles at full spatial resolution which are then re-mapped onto a regular 0.05° grid.

To generate hourly synthesis at rounded hour H all primary workfiles within the time range $[H-30, H+20]$ are used (4 workfiles for Meteosat and 6 for GOES-E). There is no interpolation and the hourly value attributed to a given pixel is the best available in the time frame, the best being selected based on criteria such as QL or time difference from rounded hour.

Hourly synthesis are then re-mapped as follow: Each quality level is re-mapped separately using a nearest neighbour approach. This results in four fields (QL 2, 3, 4 and 5) at a 0.05° resolution which are combined together giving preference to the higher QL.

5 Single Sensor Error Statistics

The SSES are observational error estimates provided at pixel level as a bias and standard deviation as per GHRSST GDSv2 requirements. They shall be provided per pixel and if possible independently of the QL.

Nowadays for operational SST processing the SSES bias and standard deviation are calculated once for each quality level from analysing differences between full resolution satellite SSTs collocated with drifting buoys available on operational matchup data set. For more information about how this dataset is constructed, please refer to section 6. This process do not give SSES independent of QL and SSES values are static.

While this is not ideal, SSES provided gives an estimate of the error with respect to drifting buoys measurements which is useful for application such as data assimilation.

6 Continuous control and validation plan

6.1 Control

The aim of a continuous control is to perform in near real time (immediately after the production of SST primary workfiles) relevant check to detect a potential problem in the functioning of the chain. The control is performed routinely and does not require in situ data (contrary to the validation, see section 6.2).

It consists in a series of maps and graphics informing about the successful development of such and such step of the processing chain. The control is performed outside the operational environment, on the workfiles and is not visible to external users. The main steps/variables monitored are listed bellow:

- Comparison to other sources of SST, in particular the Canadian Meteorological Center SST analysis.
- Monitoring of the environmental conditions: SST (analysis), water vapour, solar and satellite zenith angles, wind.
- The adjustment step: in particular we control that the adjustment reduces the differences between observed and simulated BTs.
- The SST correction: we make sure the SST correction is performing well and reduces the differences between retrieved SST and guess SST.

Figure 5 shows an example of the temporal evolution of the difference between simulations and observations before and after adjustment. During night-time, the adjustment brings the difference from approximately 0.5K to near zero on average. This is the expected behaviour. During day time one would expect a non-zero average due to diurnal warming of the surface.

6.2 Validation plan

By opposition to the control, the validation does require external sources of data and synthesis of the results will be available for users of the products through the OSI SAF web site.

6.2.1 The Matchup DataSet (MDS)

All validation procedures require a MDS has been elaborated. In an operational prospective, the MDS gathers in situ SST measurements from ship, moored buoys and drifting buoys available through the Global Telecommunication System (GTS). Collocated full resolution satellite information is added in a 3 hours time frame around the measurement. It consists in all the variables included in the intermediate workfile extracted in a box around the in situ measurements. The MDS for day d is currently elaborated with a five days delay (d+5) to ensure all in situ data are available through GTS. For the purpose of operational validation:

- Only drifter and moored buoys are considered.
- Only the central SST of each box is used.
- Night-time and day-time algorithm are validated separately.

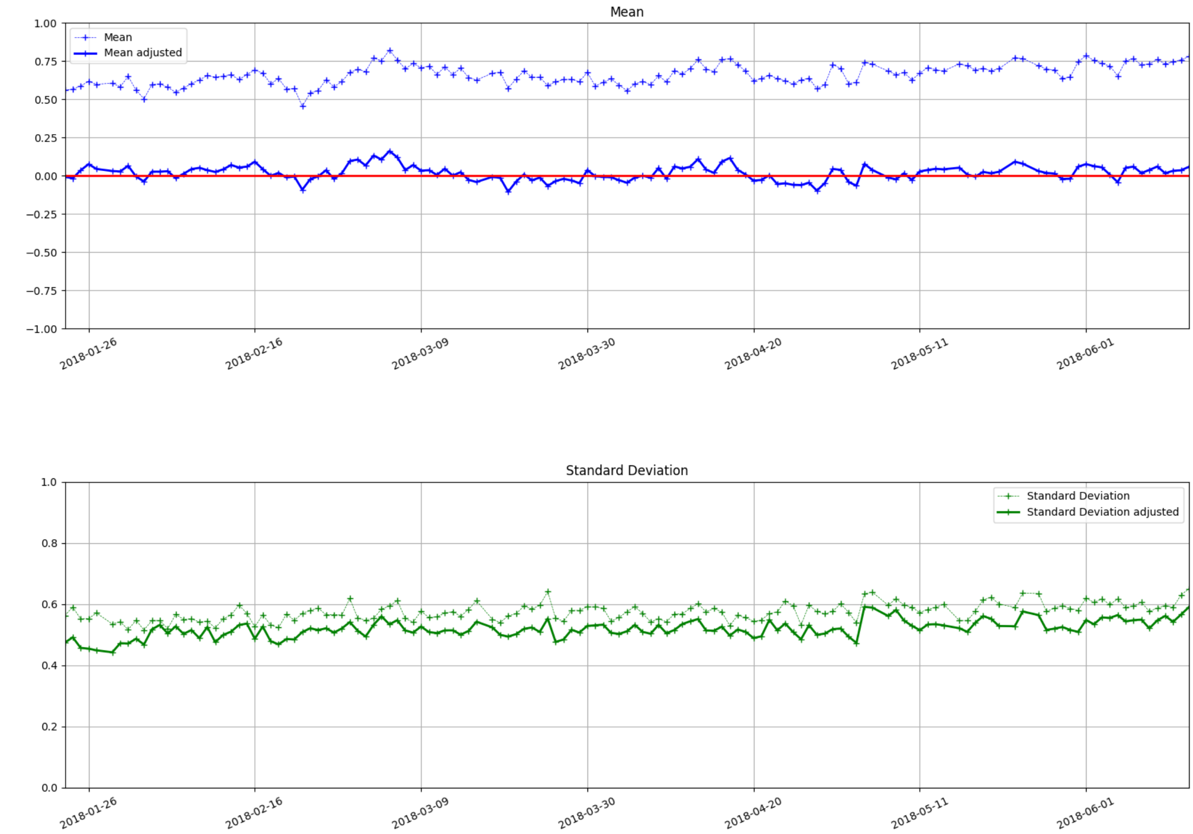

Figure 5: Control of the BT adjustment for 8.5μm channel. Temporal evolution of the difference, in K, between simulated BT and observed BT (solid lines with crosses), and between simulated adjusted BT and observe BT (dotted line with crosses). The top plot represents the mean of the differences and the bottom plot represent their standard deviation.

6.2.2 Statistics

To ensure the product satisfies the requirements of [AD.1], statistics are computed routinely (in delayed mode) and manually. They include normal and robust statistics:

- Mean and Standard Deviation of the difference between the retrieved SST and the measurements.
- Median and Robust Standard Deviation (**?**) of the difference between the retrieved SST and the measurements.

Normal statistics are displayed on OSI SAF website, a more thorough analysis is performed and reported in the half yearly operations report on OSI SAF activities. A validation report dedicated to this SST product is also provided as part of the Operational Readiness Review.

The main characteristics of the validation are:

- Global and regional analysis.
- Productions of maps of binned statistics (on a regular grid and for a time frame). Figure 6 shows a sample of monthly average difference.
- Analysis for different selection criteria, for example based on the quality level or wind speed, etc...

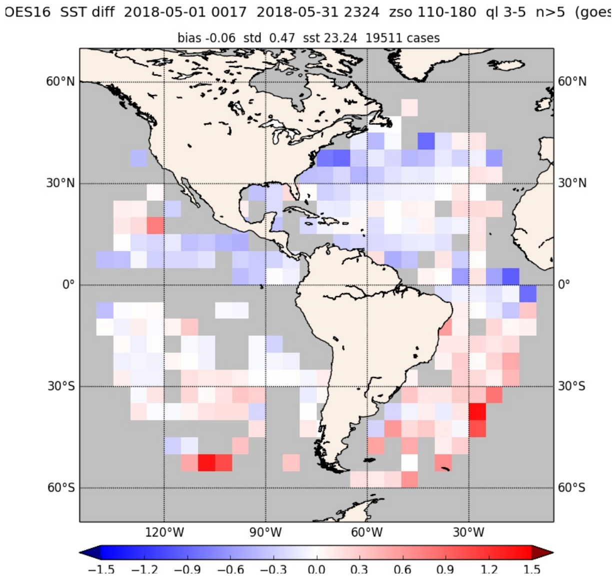

Figure 6: Example of maps of binned night-time differences $\mathrm{SST}_{\mathrm{GOES-16}} - \mathrm{SSTinsitu}$ *for the month of May 2018.*

- Analysis of the dependence of the error with respect different variables: latitude, SDI, satellite zenith angle, etc... (see example provided by Figure 7)

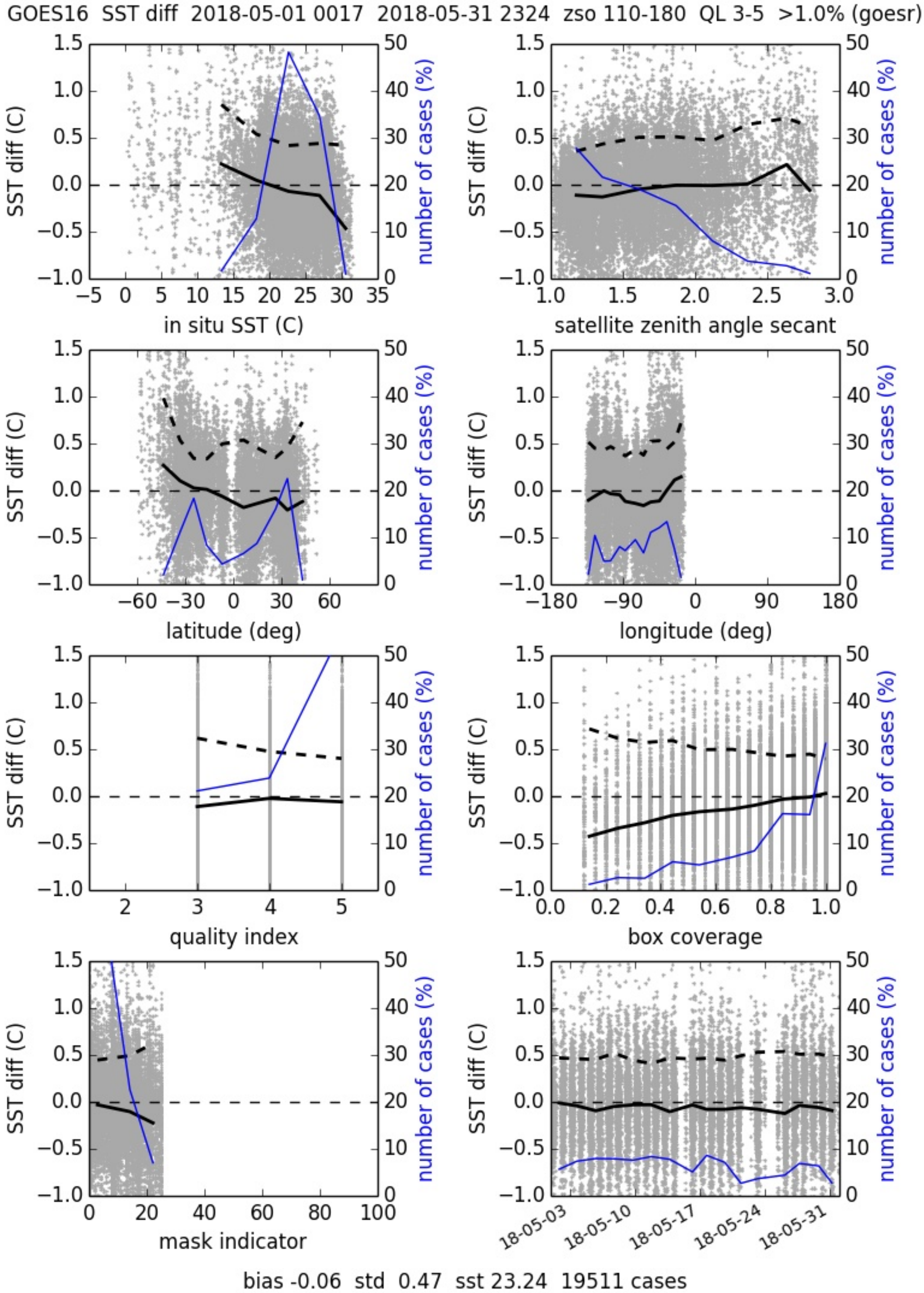

Figure 7: Example of dependence plots night-time differences $\mathrm{SST}_{\mathrm{GOES-16}} - \mathrm{SSTinsitu}$ *for the month of May 2018.*