



Sea-ice Surface Temperature Retrieval and Validation for Copernicus Sentinel-3 Sea and Land Surface Temperature Radiometer - EUMETSAT ITT No. 215580

Product Validation Plan - Including IST performance against In Situ observations, cloud mask performance and inter-comparison between Sentinel-3 SLSTR A and B IST data.

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Product Validation Plan

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Abstract

The recommended algorithms are validated with respect to accuracy, as well as with respect to possible systematic and structural biases following QA4EO guidelines [AD-5].

Validation data sets are identified and agreed with EUMETSAT at Kick Off, including satellite observations from comparable products and missions.

A Product Validation and evolution Report (PVR) will be prepared describing the findings, from using this document as guideline. The PVR will contain full details of tests, evaluation and their results.

Document change record

Version	Date	Author	Description
V1.0	February 5th 2019	Jacob L. Høyer	First version
V2.0	March 28 2019	Jacob L. Høyer	Answers to RIDs
V2.1	April 10 2019	Jacob L. Høyer	Missing figure added
V2.2	May 1 2019	Jacob L. Høyer	Document reference number added.
V2.3	December 19 2019	Gorm Dybkjær	Minor revision.

Applicable Documents:

[AD-1] Requirement Baseline Document (RB, D4)

[AD-2] Input Output Data Definition Document (IODD, D6)

[AD-3] Algorithm Theoretical Basis Document – working paper (ATBDv1, D7.1)

[AD-4] Project Proposal

[AD-5] QA4EO documentation (<http://www.qa4eo.org>).

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1. Acronyms and abbreviations

AVHRR	Advanced Very High Resolution Radiometer
AWS	Automatic Weather Station
CCI	Climate Change Initiative
CDR	Climate Data Record
ESA	European Space Agency
EUMETCast	EUMETSAT's primary dissemination mechanism
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
Felyx	Free, open source, software system for the analysis of large Earth Observation datasets
GDS	GHRSSST Data Specification
GHRSSST	The Group for High Resolution Sea Surface Temperature
IMB	Ice Mass-balance Buoy
IST	Ice Surface Temperature
L2, L3, L4	Level-2, Level-3, Level-4
LST	Land Surface Temperature
Metop	Meteorological Operational (EUMETSAT)
MIZ	Marginal Ice Zone
MIZT	Marginal Ice Zone Temperature
MODIS	Moderate Resolution Imaging spectroradiometer
MUDB	Match-Up Data Base
NWP	Numerical Weather Prediction
OSISAF	Ocean and Sea Ice Satellite Application Facility
OSI-205	OSISAF operational L2 IST product based on Metop AVHRR and VIIRS data
PROMICE	Programme for Monitoring of the Greenland Ice Sheet
QC	Quality Control
RTTOV	Radiative Transfer for TOVS (TIROS Operational Vertical Sounder)
SAMS	Scottish Association for Marine Science
SLSTR	Sea and Land Surface Temperature Radiometer
SOW	Statement of Work
SST	Sea Surface Temperature
VIIRS	Visible Infrared Imaging Radiometer Suite
WBS	Work Breakdown Structure

2. Introduction

Validation activities will be carried out to test algorithm performance. These activities will cover both Northern and Southern high latitude regions and different aspects of performance, as well as temporal and geographical dependencies of bias and standard error. In this context, the high latitudes are understood as the regions poleward of 50 degrees latitude. Based on recommendations in the review and requirement report [AD-1], 11 IST algorithms are selected to be tested for performance. These algorithms are described in the ATBD version 1 [AD-3]. The final product Validation Report will lead to the recommendation of one algorithm, or compound algorithm, to represent the final SLSTR IST algorithm. The validation activities will cover a one-year period from August 1 2016 to July 31 2017.

Beside the traditional validation, the validation statistics is also stratified into in situ platform type. Traditional in situ temperature measurements over sea ice often are erroneous, mainly due to snow covering the instruments. Results are therefore discussed in relation to the representativeness of each observation type.

The validation activities also include comparisons against other satellite data and Numerical Weather Prediction model data. In addition, an inter-comparison between IST derived for SLSTR-A and SLSTR-B will be carried out for a half-year period from January 2019 to June 2019.

The SLSTR IST theoretical retrievals of uncertainties will also be validated in accordance to the real performance, i.e. real errors must agree within bins of theoretical uncertainties.

The official SLSTR cloud screening products included in the products (the Basic and Bayesian) will be validated to the extend it makes sense. These algorithms are not dedicated for ice covered areas, and cold TOA radiance is to some extent defined as cloud in these algorithms, thus by default classifying cold ice surfaces as cloud. In addition, a cloud screening inter-comparison will be performed between two additional cloud products, the SLSTR sea ice cloud screening algorithm [Liberti et al., 2017] and the cloud screening algorithm from University of Leicester [Ghent et al., 2017]. Performance of all 11 IST products are tested using various combinations of cloud screening products.

3. Validation metrics and definitions

The following metrics are used throughout this document to assess the performance of the algorithms:

Discrepancy: The difference between the result and the validation value.

Bias: The mean value of the discrepancy.

Standard deviation of differences: The standard deviation of differences between the satellite and reference.

The following definitions have been used throughout the document:

Ice Surface Temperature (IST): The temperature measured by an infrared radiometer typically operating at wavelengths 3.7-12 μm (chosen for consistency with the majority of infrared satellite measurements) that represents the skin of the snow and ice temperature.

Calibration: The process of quantitatively defining the system response to known, controlled system inputs.

Validation: The process of assessing by independent means the quality of the data products (the results) derived from the system outputs.

4. In situ observations

Fiducial Reference Measurements (FRM, <https://earth.esa.int/web/sppa/activities/frm>) are defined as independent, fully characterized, and traceable ground measurements that follow the guidelines outlined by the GEO/CEOS Quality Assurance framework for Earth Observation [AD-5]. FRM delivers the required confidence in data products, in the form of independent validation results and satellite measurement uncertainty estimation, over the entire end-to-end duration of a satellite mission.

Within the FRM4STS project (www.frm4sts.org), thermal infrared radiometer (TIR) observations have been validated in the laboratory and in inter-comparison campaigns that have been conducted over water land and ice. Together with the ability to perform post-deployment calibrations, the TIRs are thus making a very good source of FRM for surface temperatures. When performing validation of satellite retrieval algorithms it is therefore desirable to use FRM in situ observations to perform a credible validation of the SST and IST products. As discussed within the FRM4STS project (Fox et al., 2018) the sea ice areas unfortunately have very limited FRM TIR observations that can be used. Other types of observations that are not classified as FRM observations will therefore also be used for the algorithm validation.

The IST in-situ observations will be gathered from various operational data streams and research projects. An automatic quality control procedure has been developed specifically for IST applications within the ESA FRM4STS project [Høyer et al., 2018] and further developed and used within the OSI-SAF. The QC includes 16 quality tests, with sanity, self-consistency and buddy checks. It is frequently updated and currently containing data up to 2018-01-01. The observation types within the in situ observation database are (Not all types are available within the agreed SLSTR IST validation period):

- Conventional air/ice temperatures from GTS drifters (DMI and ECMWF) covering global sea ice.
- Thermometric surface temperatures from IMB (SAMS, BAS, CRELL) covering Arctic Ocean, Fram Strait and few from the Southern Ocean.
- Radiometric surface temperatures from ship and aerial campaigns (IceBridge, DMI/LOMROG, POLARSTERN/AWI, Tara and MET Norway, 4 winters of DMI-AWS deployments on the fiord of Qaanaaq, NW Greenland).
- Surface and air temperature observations from various scientific campaigns, like SST observations from drifting buoys and Argo floats, from the Coriolis archive.
- Polar Automatic Weather Stations (AWS), some only recording 2 m temperatures, others measuring radiation balance, including estimated skin temperatures and fractional cloud cover.

All the IST in-situ observations have been read and formatted into a common NetCDF format. Along with the data processing, an inventory list will be maintained with all relevant information about the in-situ observations, such as data policy, timeliness, data distribution, spatial and temporal sampling. Uncertainty estimates will also be provided for each type of in situ observations. The distribution of applied in situ data are shown in figure 1, where each 5th data point is plotted on a map and the monthly data frequency is shown in histogram for Northern and Southern hemispheres, respectively.

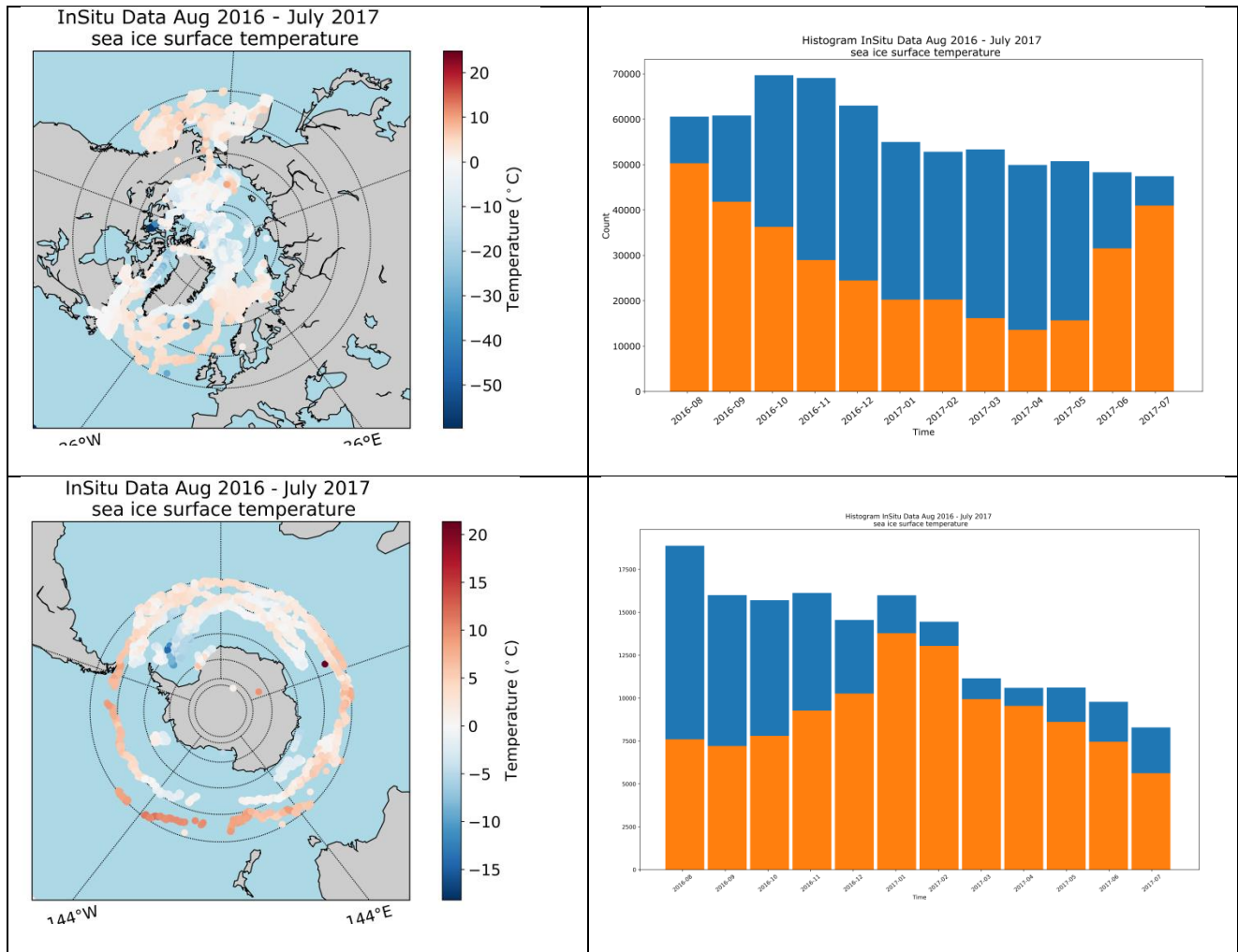


Figure 1 The spatial and temporal coverage of the applied in situ observations for the period August 1st 2016 to July 31st 2017. Top row is spatial distribution of NH data (left) and monthly distribution (right), where blue columns are temperature data lower than 0 °C and orange columns are observations warmer than 0 °C. Bottom row is the corresponding data distribution for SH.

5. Match-Up Data Base

For the calibration and validation of the retrieval algorithm, a match-up database (MUDB) is generated, including the satellite brightness temperature observations matched up against in situ observations. The spatial and temporal criteria for matching an in situ observation with a satellite observation are 5 km and 3 hours, respectively.

The MUDB shall include the surrounding 401401 SLSTR pixels around SHIP observations and temporally averaged IceBridge data (averaged to 30-second observations). For drifter buoy observations and other drifting platforms and AWS locations, the corresponding surrounding SLSTR pixel matrix is 21x21 pixels.

The MUDB will collect and assemble the following information, where available:

- In situ observations from Automatic Weather Stations (AWS), Ice Mass Balance Buoys (IMBs), drifting buoys and Operation Ice Bridge of:
 - Temperature (T2m and Tskin from sensor)
 - Radiometric Tskin
 - Wind speed
 - Humidity
 - Radiation (in/out, Long/Shortwave)
 - Cloud cover
- IST/airTemp in situ measurements from DMI in situ db:
 - Quality_flags
 - Including any quality level (1-5). Will be determined from the 'quality_flag'
 - Ice bridge data averaged over 1 km with center of the 1 km path as position. Quality level (1-5) will be determined from the variance of the temperature within the 1 km path length (large variation resulting in low quality and vice versa)
- SST observations from the Coriolis data archive poleward of 60 South and 60 North
- SLSTR data from Eumetsat L1 (all RBT) and L2 (WCT and WST) either NTC or reprocessed data. Both Nadir view and oblique view data are included
 - All relevant channels for IST/SST and cloud screening
 - Official SLSTR L1 cloud parameters from Basic and Bayesian cloud masks
 - Any relevant noise/quality data that are available and relevant
 - Sun, satellite and view geometry
 - All SSTs from WCT and WST (including quality indicators and sun-satellite-view geometry)
 - NWP (25 layers from SLSTR data stream) for RTTOV processing
 - SLSTR IST recommended from the requirement baseline document and ATBD v1 [AD-1 and AD-3] will subsequently be calculated and added
 - Atmospheric humidity from the MHS instrument (Level 2)
 - Simulated observations
 - Native and cloud masks based on the official SLSTR cloud-over-ice ATBD [Liberti, G.L, 2017] Requirements are SLSTR level 1b, and surrounding 3x3 pixels in some cases
- Alternative cloud-screening procedure developed at University of Leicester, based on SLSTR data and simulated TOA TBs (see section 5.5.6) [Ghent, D., 2017]. Daily sea-ice concentration (Operational product OSI-401-b)
- Metop IST (operational product OSI-205)
 - IST ('surface_temperature')
 - IST uncertainty (3 variables)
 - L2p_flags (ghrsst variable)
 - Processing_flags

- Quality_level
- Probability_of water
- Probability_of_ice
- View and sun geometry

6. Uncertainty and sampling effects

Due to the nature of the ice surface temperature observations, the establishment of an IST FRM to be used for satellite climate data record validation must include both assessment of the sensor performance and the representativeness effects due to spatial and temporal variability. In particular, the vertical transformation of the ice drifting observations to the skin IST is very different if the sensor is 20 cm above the sea ice or covered with 5 cm of snow, this is due to the large vertical temperature gradients within the snow pack during winter. To obtain a reliable validation results, the magnitude of all these effects needs to be assessed. A first assessment was performed in the ESA project FRM4STS (Høyer et al., 2018), where campaign in situ observations from the sea ice were used to estimate the different numbers.

If we assume all the components to have a Gaussian distribution and not to be correlated, the satellite versus in situ difference between a satellite and in situ observation is given as:

$$\sigma_{SAT-situ} = \sqrt{\mu_{SAT}^2 + \mu_{situ}^2 + \mu_{\Delta x}^2 + \mu_{\Delta t}^2 + \mu_{\Delta z}^2}$$

Where μ_{SAT} and $\mu_{in situ}$ are the uncertainties on the satellite observations and in situ observations, respectively. $\mu_{\Delta x}$, $\mu_{\Delta t}$ and $\mu_{\Delta z}$ are the sampling contributions introduced by the geophysical variability associated with point versus footprint (Δx), difference between satellite and observations time (Δt) and the difference between the vertical level of observations (Δz).

Following Høyer et al., 2017 we assume that the uncertainty on the TIR observation is 0.2°C, whereas the uncertainty on the buoys and weather station observations is 0.05°C.

The uncertainty and sampling budget estimates derived within FRM4STS are shown in table 1 for different spatial and temporal sampling differences.

Table 1: Estimates of the components in the uncertainty budget, when comparing the satellite IST observations against in situ observations (Taken from Høyer et al., 2018). T_{Buoy} represents the temperature at the snow/ice interface.

Δx (km)	Δt (min)	Δz (m)	μ_{situ} (°C)	$\mu_{\Delta x}$ (°C)	$\mu_{\Delta t}$ (°C)	$\mu_{\Delta z}$ (°C)	$\sqrt{\mu_{situ}^2 + \mu_{\Delta x}^2 + \mu_{\Delta t}^2 + \mu_{\Delta z}^2}$ (°C)
1.0	10	IST_{skin}	0.2	0.12-0.25	0.34	0	0.41-0.47
1.0	30	IST_{skin}	0.2	0.12-0.25	0.71	0	0.75-0.78
1.0	60	IST_{skin}	0.2	0.12-0.25	1.11	0	1.13-1.16

1.0	10	T_{2m}	0.05	0.12-0.25	0.34	1.45 - 2.38	1.49-2.42
1.0	30	T_{2m}	0.05	0.12-0.25	0.71	1.45 - 2.38	1.62-2.50
1.0	60	T_{2m}	0.05	0.12-0.25	1.11	1.45 - 2.38	1.83-2.64
1.0	10	T_{buoy}	0.05	0.12-0.25	0.34	3.27 - 4.95	3.29-4.97
1.0	30	T_{buoy}	0.05	0.12-0.25	0.71	3.27 - 4.95	3.35-5.01
1.0	60	T_{buoy}	0.05	0.12-0.25	1.11	3.27 - 4.95	3.46-5.08

The table above demonstrates the challenges involved in calibrating and validating satellite IST products using in situ observations. When using traditional observations, such as T_{2m} and T_{buoy} for satellite versus in situ matchups, the cumulated effects of the components not associated with uncertainties in the satellite IST retrievals can reach more than 5°C. It is also clear from the table that the most suitable FRM observations for satellite validation are traceable radiometric observations from an FRM radiometer measuring with sub-hourly intervals (e.g. 1 minute).

Note that these estimates are for sea ice covered areas. In the mixed ice and ocean regions, the gradients in the surface temperatures are significantly higher than over sea ice only or open ocean. This will be represented through an elevated spatial sampling uncertainty component

7. Product validation

7.1 Organisation of validation activities

The validation activities described in this document includes the following tasks:

- SLSTR IST validation against in situ observations, using the MUDB
- Inter-comparison between SLSTR IST and Metop IST products
- Inter-comparison of IST retrieval estimates from SLSTR-A and SLSTR-B
- Evaluation of the official cloud mask products from the SLSTR L1B data stream (Basic and Bayesian). In addition, the performance of the cloud masks developed specifically for sea ice areas (Liberti, 2017) and the cloud mask for land snow and ice covered areas (Ghent and Sembhi, 2017) will be evaluated, and compared to the two SLSTR ice masks

Different analysis procedures will be applied, dependent upon the type of validation and verification that will be carried out. Three procedures will be applied:

- **Point versus pixels:** This method will be used to compare satellite and in situ observations in regions where in situ observations are available
- **Time series:** This method will be used for inter compare time series of different products in regions where no in situ observations are available. The procedure is used to obtain information about the performance of the satellite products in data sparse regions
- **Subjective verification:** For selected cases, it can be very beneficial to perform a subjective and visual inspection of different products for a larger area (e.g. 400x400 km). This is particularly the case for the cloud mask verification, where the spatial texture of the mask contains important information about the performance of the cloud mask

7.2 Key selection criteria for best IST algorithm

The key criteria used for evaluating the various IST algorithm performances are:

- **Bias:** The systematic difference from ground truth. This will be assessed using the MUDB to determine the systematic differences from validation data
- **Standard deviation:** the standard deviation will be used to assess the variability around the Bias for the satellite versus in situ matches in the MUDB
- **Stability:** The inter-comparison time series will be used to assess the performance of the IST products in the different seasons
- **Generality:** The degree to which an algorithm is adaptable to the other sensors such as SLSTR B, C and D

The key criteria used for evaluating the cloud masks are:

- **Contingency table:** To calculate the degree of agreement between the cloud screening procedures. Threshold values will be used to define cloud/no-cloud for the probabilistic cloud products
- **POD:** Probability Of Detection (POD) for both cloudy and cloud-free conditions
- **FAR:** False Alarm Rate (FAR) for both cloudy and cloud-free conditions
- **Hit Rate:** Hit rate (HR) for the cloud detection

- **Spatial texture:** The performance of the cloud masks from visual inspection of selected scenes for cases of special interest

The following sections describe the specific details of the validation and verification within the different tasks.

7.3 SLSTR IST performance against observations

The SLSTR IST product(s) will be validated using the MUDB according to the general validation plan. The measures for validation and inter-comparisons will be standard deviation of differences (STD) and mean bias.

The following validations against in situ observations will be carried out:

- SLSTR IST comparisons to in situ observations. Separate validation statistics will be derived for SLSTR IST against traditional IST buoys and dedicated surface temperature measurements (e.g. radiometer and Ice Mass –balance Buoy measurements)
- Satellite time series will be compared at selected stations to evaluate capability for diurnal temperature variation monitoring
- The satellite IST differences will be assessed with respect to:
 - a) IST/SST retrieval quality flags
 - b) Sun and satellite view geometry
 - c) Surface temperature
 - d) Seasons
 - e) Sea ice concentration
 - f) Temporal homogeneity
 - g) Hemisphere
 - h) Probability of water/ice/cloud
 - i) Observed cloud cover

A full validation of the SLSTR SST products for the Arctic will not be carried out here, but the WCT and WST SLSTR SST products will be evaluated as approaching the sea ice. The aim of the evaluation is to ensure a seamless transition from the open ocean SST retrievals and the sea ice IST. This validation will consist of comparison of the SST and IST retrievals using relevant campaign data from e.g. Operation IceBridge data.

7.4 SLSTR IST inter-comparison with NWP and Metop IST data

A comparison will be carried out for the SLSTR IST products against NWP surface temperatures and Metop IST products included in the MUDB.

The following comparisons with other data will be carried out:

- SLSTR IST will be inter-compared with Metop-IST from OSISAF (OSI-205)
- The satellite time series will be compared at selected stations to evaluate the capability for diurnal temperature variation monitoring.
- Time series of the two satellite IST products will be compared with respect to:
 - a) SLSTR and Metop retrieval quality flags

- b) Sun and satellite view geometry
- c) Surface temperature
- d) Seasons
- e) Sea ice concentration
- f) Temporal homogeneity
- g) Hemisphere
- h) Probability of water/ice/cloud
- i) Observed cloud cover
- The SLSTR IST performance will be assessed with respect to:
 - a) Total Column Water Vapour (TCWV) from NWP

7.5 SLSTR IST – inter-comparison between Sentinel-3 A and B

This validation will include time series inter-comparison of Sentinel 3 A and B IST products at selected uniform locations, i.e. definitely ice surfaces. The locations will be chosen to represent both hemispheres and at different latitudes to be as representative as possible. The period of inter-comparison will be from January 2019 to June 2019 and will be carried out to assess any biases between the two products, but also to analyse the daily variability.

7.6 Cloud mask evaluation and inter-comparison

The Basic and the Bayesian cloud mask included in the SLSTR L1B data products and the two additional probabilistic cloud masks for ice infested areas by Liberti (2017) and from University of Leicester (Ghent and Sembhi, 2017), will be intercompared. It is commonly known that undetected clouds are the single most important error component for satellite IST performance (Dybkjaer et al., 2012), (Hall et al., 2012). Cloud screening is more complicated over ice than over ocean because of the spectral and structural resemblance between ice and snow covered surfaces. It is therefore crucial to verify the performance of these cloud masks. Cloud screening procedures are, however, not the focus of this project, but we will evaluate the IST performance in relation to all four included cloud products. The cloud evaluation will comprise a visual and subjective comparison of the four individual cloud tests for selected geographical areas. In addition, a direct comparison will be performed using calculated cloud cover from sites with in situ cloud fraction estimates, i.e. the PROMICE Automatic Weather Stations on and at the rim of the Greenland Ice sheet. Based on the outcome of these tests we will provide recommendation for EUMETSAT regarding the individual cloud mask performances and potential synergy effect of using several of the cloud tests sequentially.

7.7 Evaluation of uncertainty

The SLSTR IST retrievals will be accompanied by an estimate of the IST retrieval error through the development of an uncertainty algorithm. As a part of the product validation, the retrieval total uncertainty will be validated and verified from corresponding satellite IST estimated and most reliable in situ measurements.

In order to reduce the sampling effects (as described in Section 6), the uncertainty validation will primarily be performed against the in situ radiometric observations, where the sampling effects are minimal.

8. References

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