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Project : **FRM4SST (ships4SST: FRM4SST Phase 2)**

Title : **Traceable SST validation for CIMR**

Abstract : This document contains an overview of the current in-situ validation techniques available for SSTs measured by CIMR.

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1. INTRODUCTION

This document discusses approaches to the traceable validation of Copernicus Imaging Microwave Radiometer (CIMR) Sea Surface Temperature (SST) products, based on objectives and requirements from the CIMR Mission Requirements Document (MRD) [1].

The CIMR MRD sets demanding objectives and requirements for the total uncertainty of Level 2 Sea Surface Temperatures (SSTs) (0.2 K, 1σ) and notes the value of validation campaigns and Fiducial Reference Measurements (FRMs) to evaluate all CIMR products:

> PRI-OBJ-2: "Measure Sea Surface Temperature (SST) in non-precipitating atmospheres at an effective spatial resolution of ≤15 km, with a total standard uncertainty of ≤0.2 ±0.1 K with a focus on sub-daily coverage of Polar regions and daily coverage of Adjacent Seas"
>
> SEC-OBJ-1: "Measure Sea Surface Temperature (SST) in non-precipitating atmospheres at an effective spatial resolution of ≤15 km with a total standard uncertainty of ≤0.2 K with daily coverage of the global ocean and inland Seas"
>
> MRD-900: CIMR shall generate L2 Sea Surface Temperature (SST) products at a resolution of 15 km in the open ocean, with a standard total uncertainty of 0.2 K for 95% global coverage and sub-daily coverage in the Polar Regions and Adjacent Seas.
>
> MRD-1150: A technique for the quantification and propagation of each of the contributing sources of uncertainty in the L1a, L1b, L1c and L2 data products shall be identified in the Scientific Calibration and Validation Concept Document.
>
> *Note 1: For example, techniques may include validation campaigns using dedicated ships/aircraft, use of existing Fiducial Reference Measurements, or comparison with other satellite data.*
>
> *Note 2: In designing such techniques and associated methods, care needs to be taken with the spatial and temporal scales and correlation of the uncertainties.*

Taken together, there is a requirement to demonstrate a total uncertainty of 0.2 K in the CIMR L2 SST product. In the following sections, we explore approaches for the validation of CIMR SSTs which could satisfy these objectives and requirements. In particular, we consider in-situ SST validation measurements.

2. VALIDATION APPROACHES

For the CIMR L2 SST product, the principal route to validation will be by comparison with a set of independent SST measurements. To be effective, these measurements must be of the identical quantity observed by CIMR, have comparable spatial and temporal sampling, have well-understood uncertainties and they must be *traceable* to international standards [2], most commonly the International System of Units (SI) and the International Temperature Scale of 1990 (ITS-90) [3,4], a practical realisation of the SI kelvin temperature unit.

In general, satellite radiometer radiances, and by extension, derived products such as SST, are not directly traceable as there is no mechanism to verify the instrument calibration after launch (although traceable calibration targets are being developed for future radiometer missions [5]). Consequently, CIMR SSTs cannot be validated directly against other satellite radiometer measurements and instead must be validated directly or indirectly against in-situ SST measurements.

Currently, there are two main sources of in-situ SST measurements: thermometric measurements of SST at depth collected by buoys and profilers, and radiometric measurements of skin SST collected almost exclusively by thermal infrared (IR) radiometers, although there are also occasional deployments of microwave radiometers.

To contribute useful information to the validation process, the total uncertainties of the validation measurements, particularly any systematic components, should at least be comparable to, and preferably significantly lower than, those of the dataset to be validated. To validate a CIMR L2 SST at the 0.2 K level, a target validation measurement uncertainty budget of 0.1 K is appropriate. This budget should include not only the core validation measurements, but also any algorithms, models and ancillary data used to derive a comparison SST.

The validation systems discussed in the following subsections all generate “point” SST measurements, so spatial aliasing with the CIMR footprint is a potential problem for all of them. We discuss possible sampling approaches to accommodate spatial aliasing issues in Section 3.

2.1 Thermal infrared radiometers

Skin SSTs have been collected regularly with thermal infrared radiometers for more than 25 years. All of the active ocean-going instruments are self-calibrating filter radiometers or spectro-radiometers whose in situ radiometric calibrations are maintained by two on-board black bodies. The operating principles of these radiometers are very similar to those of their space-borne counterparts, such as SLSTR, VIIRS and IASI, though their detailed designs are optimised for operations in a maritime environment and include measures to protect against bad weather.

Thermal infrared radiometers typically measure upwelling sea surface radiances at a fixed nadir angle and downwelling sky radiances at the complementary zenith angle to correct for the small reflected sky component in the upwelling radiances. These measurements are interleaved with reference observations at two blackbodies, repeated every 1 to 10 minutes.

2.1.1 Advantages

Traceability

Infrared radiometers implement relatively pure self-calibration schemes. The internal calibration sources are placed at the very end of the measurement chain and consequently calibrated radiometric measurements are not sensitive to changing instrument properties, including the temperatures and reflectances of optical components.

With care, it is possible to build very good thermal infrared calibration sources. Surface coatings are available with high emissivities and, as diffraction effects are still quite small at infrared wavelengths, compact black body cavities can be designed with extremely high effective emissivities. Consequently, the spectral radiances emitted by well-designed blackbodies can accurately be described as Planck emission at the blackbody temperature.

There are at least two potential traceability routes for infrared self-calibrating radiometers, one through the instrument’s internal calibration black bodies and a second through an independent external calibration black body placed at the instrument aperture. This redundancy gives a robust way to validate instrument calibrations over time and to intercompare different instruments.

SST sensitivity

As the emissivity of the sea surface is very high at thermal infrared wavelengths (~ 0.99) and absorption is very low in the atmospheric window spectral regions, SSTs are very well correlated with water-leaving brightness temperatures (BTs). Typically, SSTs differ by less than 1 K from water-leaving BTs, even under clear skies. As a result, SSTs derived from upwelling infrared sea surface radiance measurements are relatively insensitive to uncertainties introduced from additional sources such as ancillary measurements and SST retrieval algorithms.

Relevance to satellite radiometers

Infrared radiometers measure skin SSTs. The skin depths of the infrared measurements (~10 µm) made with in-situ infrared radiometers are directly comparable with those from satellite infrared radiometers (e.g. SLSTR, VIIRS) and are closely related to the skin SSTs measured by microwave radiometers (e.g. AMSR-E, CIMR) slightly deeper (~100 µm) in the surface layer.

In situ infrared radiometers can measure under both clear and overcast skies.

Established measurement system and validation expertise

There is a strong established cooperative network, the International SST FRM Radiometer Network (ISFRN or "ships4SST"), of thermal infrared instrument operators with experience extending over more than two decades [6]. The network members have addressed many aspects of in situ infrared radiometric measurements including:

- Instrumentation
- Documentation covering all aspects of the measurement process, including methodologies to maintain traceability, deployment considerations and data formats
- An archive and website to provide access to the radiometer data
- Match-up and reporting tools
- Regular round-robins and intercomparisons

The radiometer community has extensive experience validating infrared satellite radiometers and more recently has validated large footprint satellite SST sensors such as AMSR-E and IASI.

2.1.2 Disadvantages

Coverage

There are relatively few active shipborne in-situ instruments, typically 10 – 15 at any one time. Geographic coverage is reasonably good, though most individual instruments operate over restricted regions (e.g. North Atlantic, Caribbean, Bay of Biscay).

Relevance to microwave satellite radiometers

Infrared radiometers cannot measure comparable water-leaving microwave radiances for level 1 comparisons and retrieval algorithm validations.

Infrared in situ radiometers cannot operate in precipitation or high seas.

As for all the in-situ validation techniques, spatial aliasing needs to be considered due to the mismatch in measurement footprints, as shown by IASI footprint analysis (see [7] and figure below).

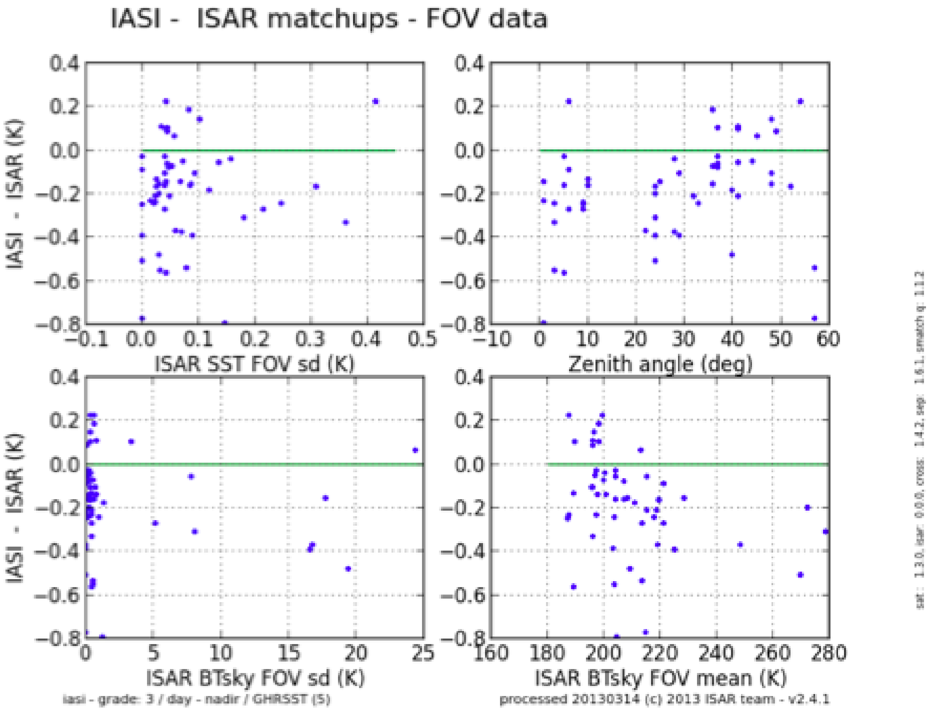

Figure 1: IASI field of view (FOV) analysis comparing various parameters against the IASI to ISAR difference. IASI has a FOV of approximately 15 km. Top left panel: IASI - ISAR mean difference vs. the standard deviation of the ISAR SST data in the IASI pixel. Top right panel: IASI - ISAR mean difference vs. the satellite zenith angle. Bottom left panel: IASI - ISAR mean difference vs. the standard deviation of the ISAR sky Brightness Temperature (BT). Bottom right panel: IASI - ISAR mean difference vs. mean of the ISAR sky BT data.

2.2 Microwave radiometers

To date, rather few in-situ microwave radiometers have made measurements over the open ocean and none have been deployed routinely. No established calibration scheme exists for MW radiometers, as it varies according to the type of instrument. However, the calibration typically follows the principles described in [8], [9] and [10]. It is a four-step procedure, where the first step uses the internal calibration references to calibrate up to a calibration reference equal to the instrument front plate. Step two considers the transmission lines between the antenna system and the radiometer, and step 3 accounts for the antenna system itself. Finally, step 4 accounts for the actual antenna orientation with respect to Earth North and true Horizontal/Vertical orientation. A detailed description of the validation is described in [8].

2.2.1 Advantages

Traceability

Microwave radiometers maintain internal calibration sources, including hot and cold loads and stable noise sources, which can provide routes to traceability for measured radiances or brightness temperatures.

The calibration of the majority of the measurement chain can be validated with matched loads substituted in place of the antenna. Liquid nitrogen cooled matched loads are a common choice.

Relevance to satellite radiometers

In situ microwave radiometers can make water-leaving polarised radiance measurements that are directly comparable with those from their microwave satellite counterparts. They are the only potential source of data for level 1 comparisons and could provide important information to validate SSTsubskin retrieval algorithms.

Retrieved in situ SSTs are potentially well matched to the satellite equivalents for algorithms based on comparable channel selections.

In situ microwave radiometers can measure under both clear and overcast skies and possibly in light precipitation.

2.2.2 Disadvantages

Traceability

Traceability is harder to demonstrate for microwave instruments. The internal calibration is applied before the final antenna or feed horn, so thermal emission from these must be removed from the measured radiances [8].

The measurement wavelengths are significant compared to the size of the instrument aperture, particularly for a compact in situ instrument, so beam patterns may be quite extensive. This makes the interpretation of upwelling radiances more challenging as information is integrated from a large range of directions.

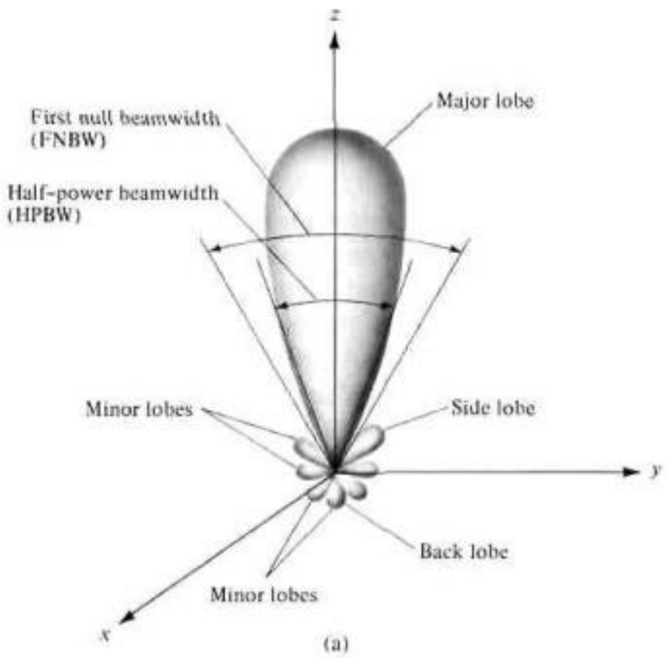

Figure 2: Image of a typical antenna beam pattern, with main lobe and small side lobes [14].

It is hard to build good external microwave black bodies to demonstrate full end-to-end calibrations in free space, especially at longer wavelengths. The emissivity of “black” coatings in this spectral region is relatively low, the coatings are quite thick and extended black body apertures are required to accept the full antenna pattern. Consequently the black body is vulnerable to temperature gradients and the achievable target emissivity is limited.

A physical retrieval is needed for a traceable SST, at least if based on the traceability of the instrument radiances, and these are challenging to develop due to the relatively low sensitivity of microwave radiances to SST (see below). Regression-based retrievals delegate SST traceability to the donor dataset.

SST sensitivity

Sea surface emissivities are lower in the microwave than in the thermal infrared regions. In addition, they are more sensitive to environmental conditions such as wind speed / surface roughness and water temperature. Consequently, SST retrieval models are more complex and the retrieved SST has an increased sensitivity to uncertainties in the emissivity model.

Established measurement system, coverage and validation expertise

There is currently no established measurement system and therefore a minimal set of data taken by in-situ microwave radiometers.

Relevance to satellite radiometers

Microwave in situ radiometers cannot currently operate in heavy precipitation or high seas due to the danger of instrument damage.

Spatial aliasing needs to be considered due to the mismatch in measurement footprints (see section 3).

2.3 Buoys

Drifting buoys and Argo floats are carried by ocean currents and measure sea temperatures in-situ, which are then transmitted to the operators. In addition, a number of moored buoys provide repeated measurements of constant points in the oceans and near to coasts. Buoys have the longest data record of any modern in situ technique. Moored buoys have operated since 1951 and drifting buoys since 1979. Argo floats were first deployed in the early 2000s.

Drifting buoy temperature measurements are taken at a nominal depth of between 10 cm and 20 cm. Argo products report temperatures at different depths: 2.5 m, 5 m, 10 m, 20 m, 30 m and deeper levels, with an initial accuracy close to 2 mK.

2.3.1 Advantages

Traceability

Argo floats experience very little fouling or mechanical damage as they spend most of their time in relatively benign conditions at depths of 1000 m. Measurements are generally stopped below the surface to avoid the fouling of the conductivity cell by surface contaminants.

Buoy networks capable of increased accuracy and stability are now being developed [11] and the instruments will be individually calibrated before deployment, which will allow improved levels of traceability.

SST sensitivity

Sensitivity to SST in the water immediately surrounding the probe is very high, though care must be taken to ensure that instrumental effects do not influence the measurements.

Relevance to satellite radiometers

Buoys and Argo floats can collect data in almost all weather conditions and sea states.

Established measurement system and validation expertise

The technology and data analysis for both buoys and Argo floats are mature and well understood. There are large communities of drifting buoy and Argo float providers, and meteorological bureaus and others have developed refined data processing methods, including blacklisting and SST correction models.

Coverage

The fleet of drifting buoys and Argo floats is large; according to the Data Buoy Cooperation Panel (DBCP) over 1,500 drifting buoys cover the seas and they provide about 90% of in situ SST data [9] and high coverage of all oceans. Typically, more than 3,000 Argo floats are active at any one time.

2.3.2 Disadvantages

Traceability

Drifting buoys and Argo floats lack the traceability of radiometer instruments. Many drifting buoys are not individually calibrated before deployment and, with very rare exceptions, neither drifting buoys or Argo floats are recovered for maintenance or re-calibration. Consequently any degradation in the quality of reported measurements can only be inferred from relative performance over time and with respect to neighbouring units.

Since drifting buoys operate at the surface, they are vulnerable to fouling and mechanical damage, and can lose their drogues.

Relevance to satellite radiometers

The measured SST is at a depth so a significant modelling correction is required, both of the instantaneous vertical temperature profile and of the time evolution of the profile. In order to use these measurements at depth to provide skin SSTs, a correction must be applied based on measurement depth, time of day and, if available, knowledge of local conditions. This introduces a higher degree of uncertainty into the SST measurement, since the measured volume of water is less comparable with the CIMR-measured skin (see Section 2.1.1).

As for all the in-situ validation techniques, spatial aliasing needs to be considered due to the mismatch in measurement footprints.

3. MATCH-UPS

To assess the quality of the CIMR SST with other measurements, such as made by infrared radiometers or buoys, the two data sets must be matched in time and space. This process of matching the data set has its own issues and uncertainties which will contribute to the perceived overall uncertainty of the validation process and therefore great care has to be taken to understand and minimise the match-up process uncertainties. The equation below shows the match-up uncertainty split into five components:

$$\sigma = \sigma_S + \sigma_T + \sigma_M + \sigma_P + \sigma_Z$$

Where σ_S represents the spatial mismatch uncertainty, σ_T the temporal mismatch uncertainty, σ_M the measurement uncertainty, σ_P the point in area sampling uncertainty, also referred to as spatial aliasing, and σ_Z the uncertainty introduced by using measurements from different depths. The two main uncertainties introduced by the match-up process are the spatial and temporal mismatch uncertainty. However for CIMR validation, the point in area sampling uncertainty becomes more important as the footprint of CIMR (5 km – 15 km) is much larger than the reference data set and also not constant, it depends on the channel combination used for CIMR SST.

This large footprint, which varies depending on channel choice used in deriving SST, needs more care than in a standard validation match-up process. A footprint analysis can be done as the reference data source will have multiple measurements in each of the CIMR pixels. Work carried on IASI [11] (see figure 1) and on AMSR-E SST data has shown that this is not a major issue, but needs consideration in areas of high SST variability, such as ocean fronts. However because the CIMR specification defines a higher accuracy of 0.2 K for SST compared to the 0.5 K of AMSR-E, the work in [11] should be revisited and verified to be applicable for CIMR.

One way of addressing the point in area sampling and spatial aliasing uncertainty is to use the footprint analysis to filter for homogeneous ocean pixels with little or no gradients in them and only use these pixels for validation.

Another possibility to assist in the footprint analysis is to use IR SST satellite sensors, such as SLTSR, VIIRS or AVHRR as a transfer standard for the reference sensor validation to CIMR. This together with the three-way uncertainty analysis between CIMR, a satellite IR sensor such as SLSTR and ships4sst data, could be a way to verify the point in area sampling uncertainty between different footprints.

A general consideration in validating CIMR has to be what SST algorithms are in use and that depending on the channel choice, the CIMR SST itself will potentially have spatial aliasing built into the product, especially when channels from the short and long wavelength end of the spectrum are combined, due to their different footprints.

4. CONCLUSION

Each of the validation approaches outlined in Section 2 brings specific benefits to CIMR SST validation.

1) In-situ thermal infrared radiometers are currently the only class of instrument that make truly traceable radiance and skin SST measurements with a physically-based SST retrieval. Global coverage is fair and there is an experienced operator community, but the number of active instruments is relatively small.
2) In situ microwave radiometers are the only instruments that potentially can measure radiances that are directly comparable with their satellite counterparts. Traceability is

possible for radiances, but is much more demanding for SST as sensitivity to the SST signal is relatively low compared with the other approaches. There are currently no routinely deployed in situ instruments.

3) Buoys and Argo floats provide by far the most extensive ocean coverage and are supported by large communities with years of experience. However, they do not measure skin temperatures and currently have very limited traceability.

All three can generate validation data under both clear and cloudy skies, but the radiometers need physical protection from rain and high sea states.

Spatial aliasing between satellite and in situ datasets is potentially an issue for all three approaches, given the relatively large size of microwave satellite footprints, but this can be addressed by multiple techniques, including homogeneity tests and infrared satellite-assisted extrapolation.

No single in situ approach provides a complete path to CIMR SST validation, but in combination they can address the most pressing issues of traceability, measurement fidelity and coverage.

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