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Compiled by : ______________________

Ruth Wilson
Space ConneXions Limited
(Project Manager)

Approved by : ______________________

Werenfrid Wimmer
University of Southampton
(Technical Manager)

Accepted by ESA: ______________________

Steffen Dransfeld, ESRIN
(ESA Technical Officer)

Distribution : Ships4SST team members

ESA

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In-Situ Sea Surface Temperature Measurements and Validation against Satellite Data: Findings from the Ships4SST Workshop

Ruth Wilson[1], Hugh Kelliher[1], Werenfrid Wimmer[2], Jacob Hoeyer[3], Tim Nightingale[4], Arrow Lee[4], Steffen Dransfeld[5], Peter Minnett[6], Nigel Fox[7], Gary Corlett[8], Jean-Francois Piolle[9]

[1] Space Connexions Limited, Harpenden, UK

[2] National Oceanographic Centre (NOC) Southampton, UK

[3] DMI, Copenhagen, Denmark

[4] STFC RAL Space, Didcot, UK

[5] ESA, ESRIN, Frascati, Italy

[6] University of Miami, USA

[7] NPL, UK

[9] Ifremer, France

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ABSTRACT

In this paper we summarise the current state of the art of using shipborne radiometers to assess the accuracy of satellite-derived SST_{skin}. Key information from the Ships4SST workshop, held on February 28 and 29, 2019, is drawn on and developed to assess what technology and networks we currently have and to outline a way forward with future Satellite data validation services to ensure that deployed *in situ* radiometers fulfil the role of validating and verifying satellite data, including the European Space Agency's (ESA) Sea and Land Surface Temperature Radiometer (SLSTR) Sea Surface Temperature (SST) data to the best of their ability.

1. Introduction

Satellite remote sensing of the Earth has become an essential tool in increasing our understanding of the climate, weather patterns and the impact of climate change. It has assisted, and continues to do so, scientists in their analysis of the Earth's climate and policy makers in the formation of policies to adapt to or mitigate the effects of climate change. For this reason, remote sensing data must be as accurate as possible as well as long-term; i.e. must be suitable for contributing to creating a reliable data series by linking different satellite sensors to common reference standards. To help achieve this, the Global Climate Observing System (GCOS) have identified a set of Essential Climate Variables (ECVs) based on the relevance of the variable in characterising the climate system, the feasibility in observing the variable on a global scale and the cost effectiveness in generating and archiving the variable data (Bojinski et al. 2014). GCOS defines an ECV as a 'physical, chemical or biological variable or a group of linked variables that critically contributes to the characterisation of Earth's climate'. To date, there are 54 ECVs, SST being one of them (GCOS, 2016). To this end, *in situ* Thermal Infrared (TIR) radiometers are deployed on vessels across the globe to collect SST_{skin} data, which are then used to validate and verify the SSTskin derived from the measurements of satellite radiometers; ensuring accuracies used for climate research, which sets very stringent accuracy requirements (see Ohring et al. 2005). SST_{skin} is a measure of the temperature within the topmost 10 µm of the surface, which is measured by TIR instruments operating at wavelengths between 3.7 and 12 µm. The Infrared SST Autonomous Radiometer (ISAR) (Donlon et al. 2008) and Scanning Infrared Sea surface Temperature Radiometer (SISTeR) (Donlon et al. 2014, section 4.2) instruments used in this project are two such TIR radiometers and they have been used in shipborne deployments since 1998 and 1996 respectively. The project has also benefitted from the submission of data from other investigators, including the SST_{skin} retrievals from the Marine-Atmospheric Emitted Radiance Interferometers (M-AERIs; Minnett et al., 2001).

The ISAR, SISTeR and M-AERI provide Fiducial Reference Measurement (FRMs), which are "the suite of independent sea-surface measurements that provide the maximum return on investment for a satellite mission delivering, to users, 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 satellite mission" (Sentinel-3 Validation Team, credit www.frm4sts.org).

Shipborne radiometric measurements provide the high accuracy surface temperature measurements (standard uncertainty <0.1 K) necessary to validate high accuracy satellite SST sensors such as the Advance Along-Track Scanning Radiometer (AATSR) that was flown on Envisat (Louet and Bruzzi, 1999; Dubock et al., 2001) and the Sea and Land Surface Temperature Radiometer (SLSTR; Donlon et al., 2012; Smith et al., 2014). Shipborne radiometers also provide a traceability route to SI (International System of Units; Taylor and Thompson, 2008) standards for satellite measurements and therefore a pathway to generate Climate Data Records (CDRs; NRC 2000; 2004) from satellite SST_{skin} retrievals (Minnett and Corlett, 2012).

To achieve robust traceability to the SI temperature scale (ITS-90), the real-time calibration of shipborne radiometers derived from their internal blackbodies is regularly verified against SI-traceable laboratory calibration targets. The traceability of both the shipborne radiometers and the laboratory calibration targets are confirmed on a regular basis through inter-comparison exercises such as the ESA-funded Fiducial Reference Measurements for SST (FRM4STS) campaign (Theocharous et al, 2016; Barker-Snook et al, 2016; Theocharous et al, 2019) held in 2016.

Shipborne radiometers provide a vitally important SI-traceable link between AATSR and SLSTR facilitating the evaluation of any offsets or trends between the two instruments. This would ideally be achieved by an overlap of the two satellite instruments for a period of six months or more. However, the sudden loss of communications with Envisat on 8 April 2012, before the launch of Sentinel 3A, prevented an overlap period. Nevertheless, because measurements were made continuously throughout the data gap, any geophysical changes in the SST_{skin} fields during the gap will have been monitored so that any such changes could be shown to be neither an attribute of AATSR nor SLSTR but a genuine geophysical change.

The latest in a long series of UK and ESA-funded contracts to support the ISAR and SISTeR deployments is known as “ships4SST”. The aim of the ships4sst service contract is to validate Copernicus Sentinel-3A and Sentinel-3B SLSTR SST data products and to promote and evolve the International SST FRM Radiometer Network (ISFRN). To this end an ISFRN workshop was held at the National Oceanography Centre (NOC), Southampton on 27-28 February 2019.

2 Current State of SST FRM Radiometer Deployments and Measurements against Satellite Data

The first international ISFRN workshop was held on 27-28 February 2019, with scientific and operational users and producers of *in situ* radiometer SST_{skin} data from the UK, Denmark, America, Australia, Italy, France and the USA attending. The aim of the workshop was to present and discuss shipborne radiometer activities, satellite SST_{skin} validation activities and results, and the experiences of the partners in the ISFRN service.

The ESA-sponsored workshop was hosted at NOC in Southampton and consisted of two days of presentations, posters and interactive sessions, designed to review progress, results and advances in deployments, calibration and validation as well as a discussion on a service roadmap. The workshop consisted of the following sessions:

- Session 1: Experiences of Radiometer Operators
- Session 2: Developing the Radiometer Network
- Session 3: Radiometer Performance and Uncertainties
- Session 4: Validation of Satellite SST Measurements
- Session 5: Software and Tools

This sequence of topics also forms the framework of this paper.

2. 1 Experiences of Radiometer Operators

The workshop began with a series of presentations from radiometer operators. Three of the instruments used by experts are the ISAR, SISTeR and the Marine-Atmospheric Emitted Radiance Interferometer (M-AERI) instruments. ISAR is a self-calibrating instrument capable of measuring in situ sea surface skin temperature to an accuracy of 0.1K. SISTeR is a chopped, self-calibrating infrared radiometer capable of measuring infrared brightness temperatures to a high accuracy of ~30mK. M-AERI is a self-calibrating, seagoing Fourier-transform interferometric infrared spectroradiometer that is deployed on marine platforms to measure the emission spectra from the sea surface and marine atmosphere. There are now 19 ISARs being or going to be deployed around the globe for various countries, as well as the SISTeR and four M-AERIs. This is encouraging as a wider network of radiometers means that a more global set of high accuracy in situ SST_{skin} data is becoming available for satellite validation.

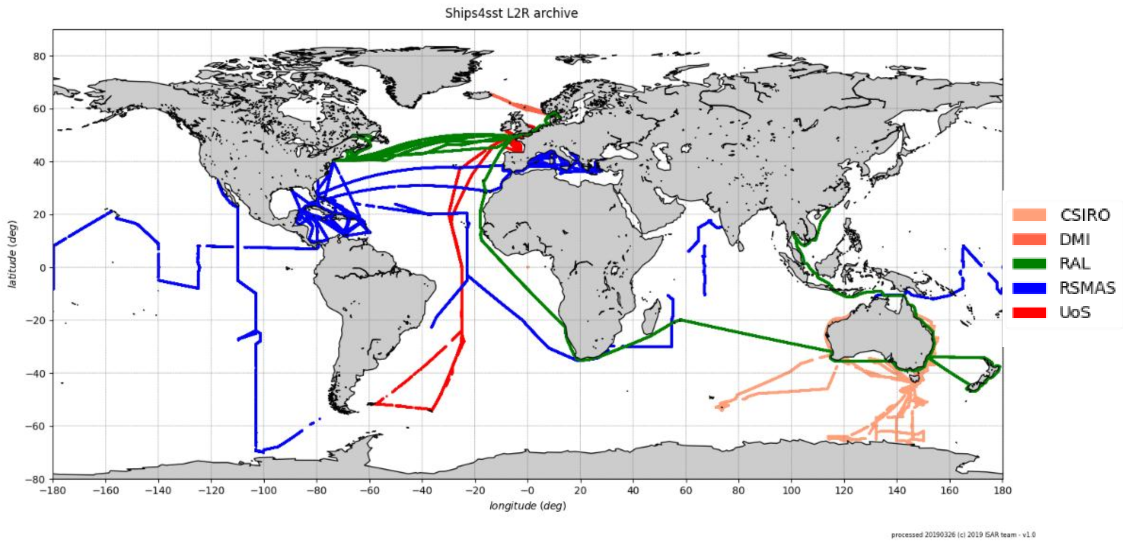

Figure 1: Tracks of ships carrying infrared radiometers the data from which are in the ships4sst archive as L2R files. The colours indicate the data provider as shown in the legend on the right hand side.

There have been 15 years of near continuous operations along the English Channel and Bay of Biscay, resulting in one of the longest SST_{skin} data records at more than 1,000,000 SST measurements. SISTeR has also been deployed on various ships since 1997, and has been on the Cunard ship *Queen Mary 2* North Atlantic and annual world cruise since 2010. It also periodically participates in radiometer round-robins organised by the national metrology laboratories to validate the calibration chain. The addition of the DMI ISAR to the service in 2017 meant that higher latitude TIR FRMs could be obtained. The motivation for this is that SST observations have elevated uncertainty in high latitudes, are subject to persistent cloud cover (that makes satellite SST measurements difficult) and in general few matching in situ observations. This ISAR deployment covers an important region across the Atlantic inflow to the Nordic seas, where there are warm and cold surface currents.

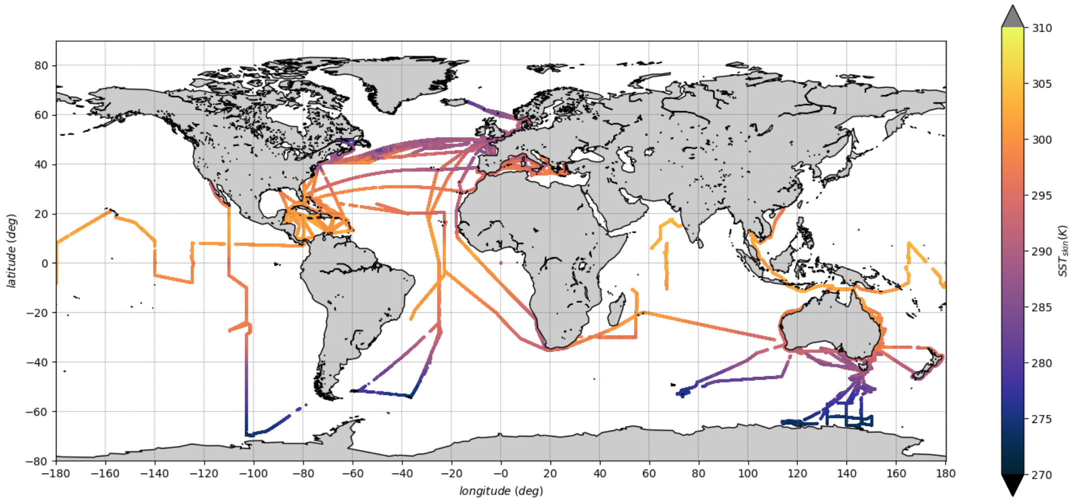

Figure 2: SST_{skin} derived from shipboard radiometers in the ships4sst data archive. The colours indicate the SST_{skin} as given on the right.

A further feature of shipborne radiometers is that they can produce per pixel uncertainties, which not only gives a degree of confidence in individual measurements, but can be validated through side-by-side inter-comparisons, such as the joint deployment of the ISAR and SISTeR instruments on the *Queen Mary 2* in 2015.

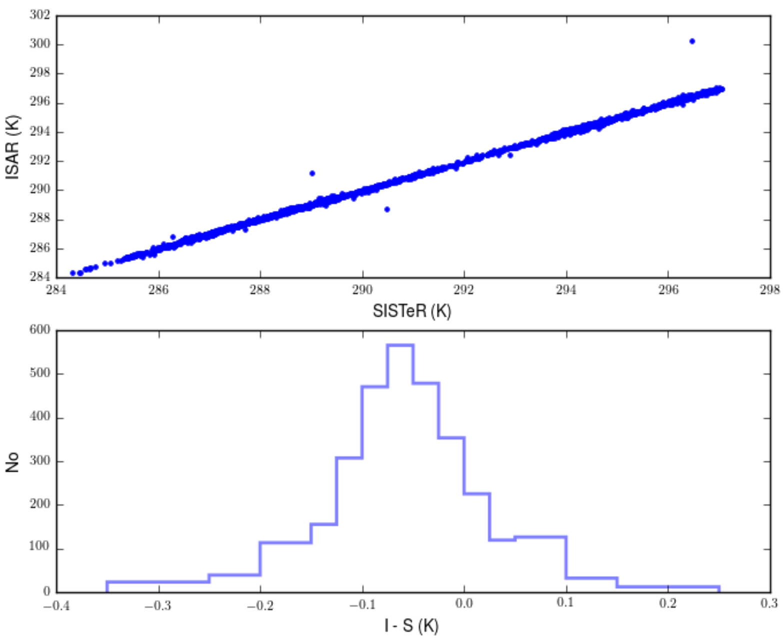

Figure 3: the ISAR and SISTeR measurements in Kelvin, showing good agreement with each other

2. 2 Developing the Radiometer Network

2.2.1 The ISFRN

The ISFRN is intended is intended to develop and promote an international network of ocean and remote sensing scientists who share a particular interest in promoting and improving the use of shipborne infrared radiometers for measuring SST_{skin} at the surface of the ocean, comparable to the retrievals made by satellite infrared radiometers. This includes operators, designers and builders of such instruments as well as the users of the data. In particular, the ISFRN aims to:

- Promote good practice in the construction and operation of shipborne radiometers
- Establish protocols, formats and standards for quality assurance of shipborne radiometer data
- Provide a single access point for the collection and dissemination of shipborne radiometer data
- Support satellite radiometer operators and the wider community in the long-term validation of satellite products
- Share knowledge and coordinate activities between Network members
- Inform the wider community about the Network's activities

An invitation to TIR operators to produce data in a standard L2R format and provide the data to the ships4sst archive was issued at the beginning of the ships4sst project and since then data have been regularly added to the archive. At the time of the ISFRN workshop, ISAR data from three countries; the UK, Denmark and Australia, SISTeR data from the UK and M-AERI data from the USA were all online and accessible via the project website. Figures 1 and 2 depict the coverage of the radiometer data in L2R files that are currently stored on the project archive, presented by data provider and as SST_{skin} respectively.

The archived ISAR, SISTeR and M-AERI data are compared with satellite data using the Felyx Match-up Database (MDB; Taberner et al, 2013) tool available at the Ifremer/Eumetsat archive facility, using the MDB analysis approach defined by Wimmer et al (2012). So far, good results have been obtained in the validation of SLSTR against the shipborne radiometers, similar to those obtained in the past for AATSR (www.atsrsensors.org). Early indications are that AATSR and SLSTR measurements are well aligned with no discernible bias between them.

2.2.2 Standards and Protocols

The ships4SST website (www.ships4SST.org) is used to host a number of important documents, two of which aim to aid the collection and dissemination of in situ radiometric data. This is the data collection protocol document and the data format document. The protocols that have been established by the ISFRN have been developed by members of the in situ radiometer community over the last several years to aid good practice in the collection of SST_{skin} data, so that data users can be sure of its provenance and quality. This is particularly important as there are no “better” SST_{skin} datasets to which the radiometer measurements can be tied, so radiometer users need to pay attention to all aspects of the measurement process to ensure traceability; the protocols document captures the practical steps necessary to implement traceable measurements. The protocols can be summarised as follows:

1. Document the SST_{skin} measurement methodology
2. Document calibration and verification methodologies
3. Verify instrument calibration *before* every deployment
4. Verify instrument calibration *after* every deployment
5. Develop an uncertainty budget for each instrument
6. Verify the uncertainty budget, particularly by comparison with other instruments
7. Ensure that documentation is accessible
8. Archive data, following good data stewardship practices
9. Consolidate and update methodologies as needed, based on your experience and that of others

The data format document describes the L2R data format that was developed by the ISFRN and is now used by three instrument types (ISAR, M-AERI and SISTeR). A common data format such as this for in situ radiometric SSTs is useful as it provides unified access for users, a guaranteed presence of basic data fields, encourages best practice (e.g. QA4EO recommendations) and implements standards across radiometer users. There are some existing in situ product specifications, e.g. the Soil Moisture Ocean Salinity (SMOS) Specification, but they have limited flexibility and lack relevant data and metadata fields. The L2R format borrows the structure of GHRSST (Group for High Resolution SST (Donlon et al, 2007) SST products so that it follows Climate and Forecast (CF) conventions (Donlon et al, 2009), implements the Attribute Convention for Data Discovery (ACDD), provides shipborne radiometer data in a consistent format familiar to the GHRSST community and is in NetCDF4. Both the protocols and data format documents can be found on the Ships4SST documents webpage (http://ships4sst.org/documents).

2.2.3 ISSI

Prior to the development of the ISFRN, the International Space Science Institute (ISSI) funded a proposal by Minnett and Corlett for a series of workshops to study the “Generation of Climate Data Records of Sea Surface Temperature from current and future satellite radiometers”. The argument was to take advantage of temperature being an SI base variable to establish the procedures to generate a satellite-derived SST CDR with SI-traceability (see Minnett and Corlett, 2012) and led to several workshops and the development of a “best practices” guidelines for calibration, at-sea deployment, data handling and distribution. Work has been undertaken to ensure that the steps to establishing SST CDRs are rigorous and well-understood by those involved in this activity and as a result has ensured SI-traceability for ship-board radiometer measurements. Figure 4 shows the ISSI-developed summary flow diagram for establishing an SST CDR, exploiting both shipboard radiometers with SI-traceable calibration, and other temperature sources, such as drifting buoys.

Many discussions and recommendations from the ISSI workshops were incorporated in chapters of: Zibordi et al., (2014), especially “Ship-Borne Thermal Infrared Radiometer Systems” (Donlon et al, 2104a), “Strategies for the Laboratory and Field Deployment of Ship-Borne Fiducial Reference Thermal Infrared Radiometers in Support of Satellite-Derived Sea Surface Temperature Climate Data .Records” (Donlon et al., 2014b), “Postlaunch Calibration and Stability: Thermal Infrared Satellite Radiometers” (Minnett and Smith, 2014), and “Assessment of Long-Term Satellite Derived Sea Surface Temperature Records” (Corlett et al., 2014).

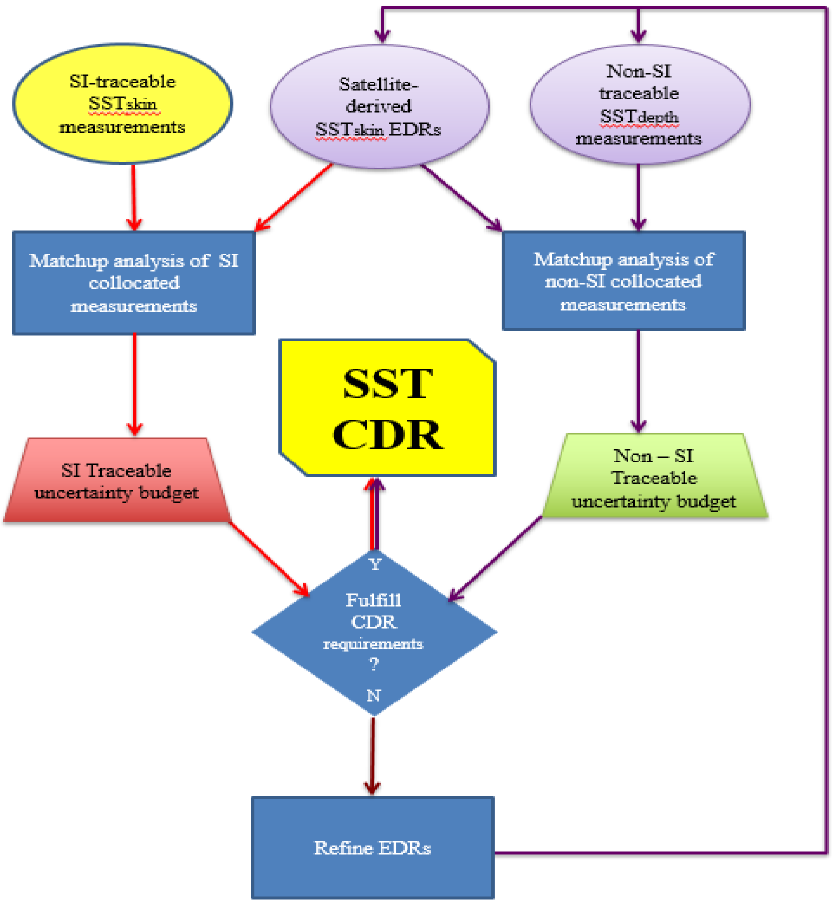

Figure 4: Flow diagram showing the traceability route for a SST CDR. The red arrows show the SI traceable links (this covers shipborne radiometers) whilst those in purple show non-SI traceable links.

2. 3 Radiometer Performance and Uncertainties

2.3.1 ISAR Uncertainty Model

FRM are required to determine the on-orbit uncertainty characteristics of satellite measurements via independent validation activities. In order to be a classified FRM not only are pre- and post-deployment calibrations required, but also a per-measurement uncertainty model. For ISAR, the model was developed on a first principle bases by analysing the components of the measurement equation (Figure 5), where the measurement equation is shown in yellow. R2T stands for radiation to temperature transformation, R_{sea} is the radiation from the sea, R_{sky} the radiation from the sky, ε the seawater emissivity, $R_{BB1,2}$ the radiation from the two on-board blackbodies, Sig_{Sea}, Sig_{Sky}, $Sig_{BB1,2}$ are the signals from the detector when viewing the sea, sky of the two blackbodies. The ISAR post processor, which was implemented following this model, produces an uncertainty value for each SST_{skin}. A detailed description of the uncertainty model can be found in Wimmer and Robinson (2016).

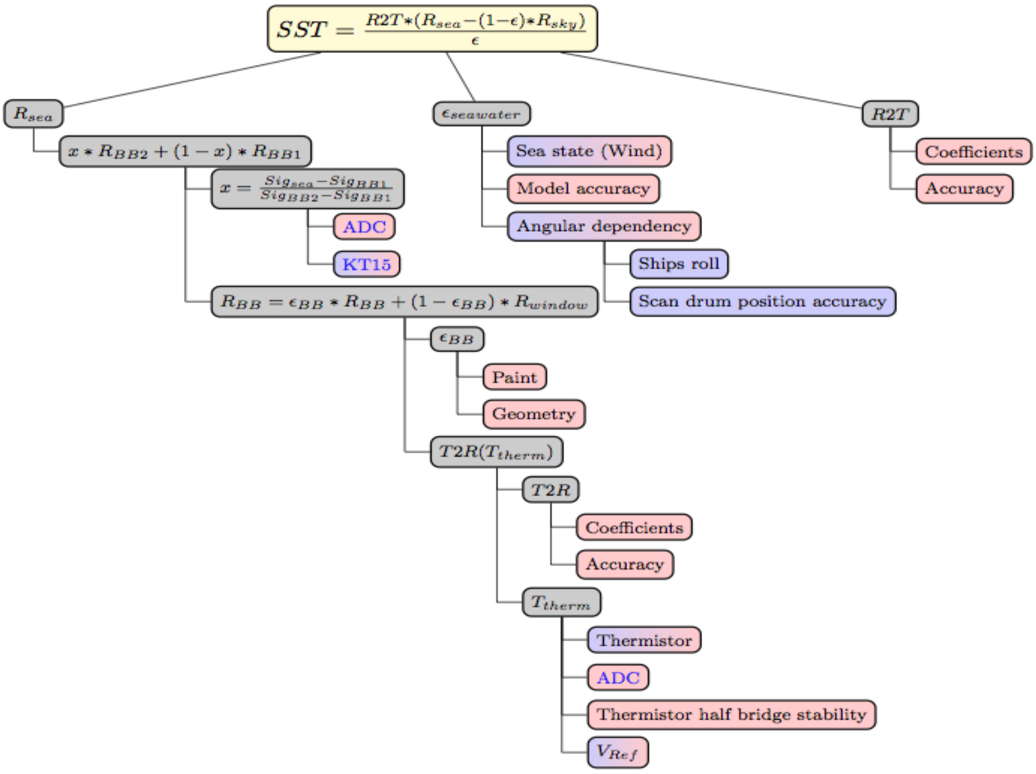

Figure 5: Schematic to illustrate the breakdown of the main elements of the ISAR SST_{skin} processor to reveal the factors that introduce uncertainty. For clarity the R_{sky} branch has not been expanded but is essentially the same as for R_{sea}. Boxes coloured in blue represent type A uncertainties, boxes coloured in red show type B uncertainties, and boxes in red and blue contain both type A and type B uncertainties. From Wimmer and Robinson (2016).

Validation of the uncertainty model is not easy to achieve, as was experienced in the uncertainty comparison experiment between ISAR and SISTeR during an Atlantic Meridional Transect (AMT) in 2018. These comparisons did show however that the instrument uncertainty is within expected parameters, that measurement uncertainties are generally overestimated and that they do not capture SST gradients well. An update to the uncertainty model is currently in progress.

2.3.2 FRM4STS

The FRM for Validation of Surface Temperature of Satellites (FRM4STS) is an ESA-funded project that aims to establish and maintain SI-traceability of global FRM for satellite-derived surface temperature validation and was established to address a CEOS request for such comparisons. To this end, comparisons between 13 different radiometers and an SI reference blackbody provided by the National Physical Laboratory (NPL) were performed during the FRM4STS project in 2016. Measurements were taken at -30ºC, 0ºC, 20ºC and 30ºC on the radiometers and the mean difference from the temperature of the NPL reference blackbody was recorded. An example of one of these experiments is shown in Figure 6.

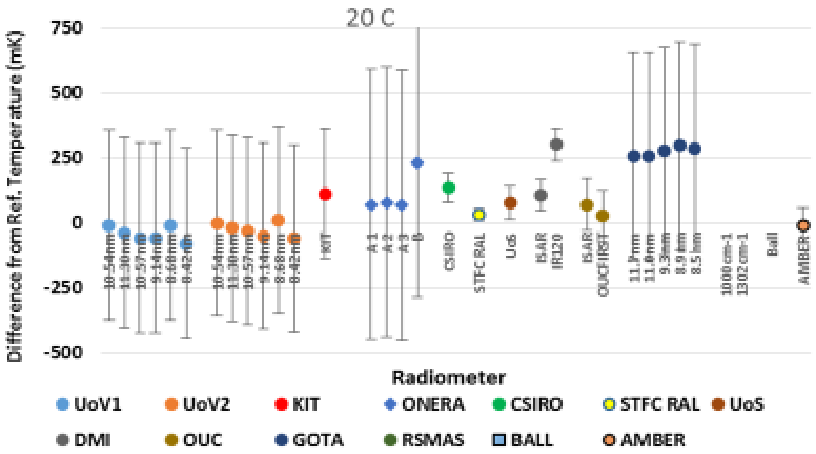

Figure 6: Plot of the mean of the differences of the radiometer readings from the temperature of the NPL reference blackbody, maintained at a nominal temperature of 20ºC. From Theocharous et al. (2016a)

Shipborne radiometers were also compared using NPL reference blackbodies over a range of temperatures; see Figure 7 for the results for a set-point of 30ºC. The results were good although there were anomalies at low and high temperatures. This showed the importance of testing the radiometers over the full range of temperatures that will be sensed by the instrument.

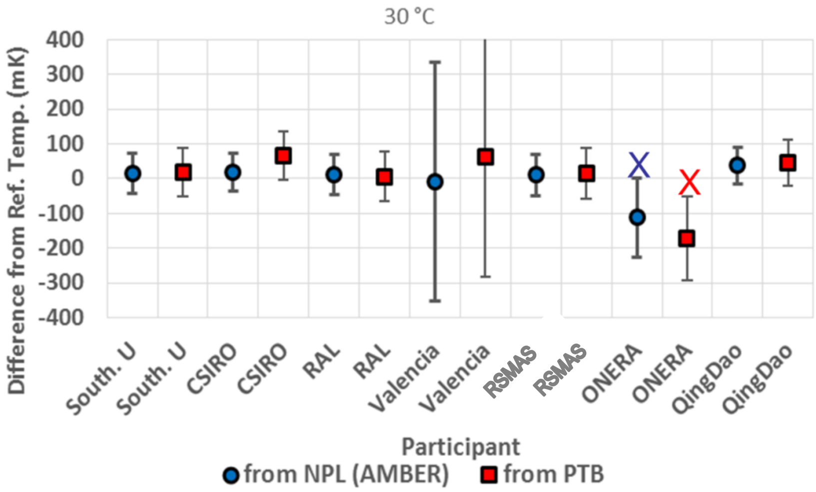

Figure 7: Difference of participant blackbody temperature at 30 ºC, measured by the NPL Amber radiometer (blue) and the PTB radiometer (red)

Comparisons such as these are key to ensuring the robustness of the instruments and to verify the accuracy of the instruments with respect to reference standards, indicating that measurements from different instruments are compatible, within the limits determined by this exercise. It is also important that results are transparent. The international consistency in ‘controlled’ conditions has been shown to be good although there is still work to do in evaluating the outliers in the observations. Uncertainty budgets for each radiometer are needed to allow for a full assessment of consistency of the results. To do this in a rigorous manner requires some effort and understanding and it is noticeable that there has been significant progress in recent years however, it is also recognised that there is a need for more training and case studies to improve uncertainty budgets further. More specific comparisons that are tailored to real world observation conditions are also being encouraged for subsequent CEOS comparison. Results of the FRM4STS lab comparisons can be found on the project website.

Some key recommendations from the FRM4STS project following on from the intercomparison exercises and workshop include:

- FRMs should be encouraged; it would be beneficial to have more sites for in situ measurements, more match-ups and more comparisons of data.
- Research is needed to examine the effects of SST_{skin} to temperature at depth transformation
- There is a desire to look at water, snow and ice temperature measurements, as well as SST.
- More training and case studies are needed on uncertainty estimation and analysis, plus “good practice” guides on measurements and instruments.
- Comparisons should account for operational conditions (low/high ambient temperature)
- Investigations into cloud detection/masking (day/night) effects on satellite data validation should be continued
- When linking satellite data to in situ data for validation, scientists should compare traceability and reference standards (i.e. do not rely on models)
- Compare retrieval algorithms (using standardised data)

- We need more SI-traceable buoys (i.e. consider triple sensors for redundancy, recoverability)
- Synergy with other observations, e.g. passive microwave and IR, should be encouraged

2.3.3 Comparing Shipborne Radiometer with in situ measurements

Assessment of uncertainty of satellite measurements involves comparison to a reference dataset, such as SST_{skin} from shipborne radiometers, subsurface temperatures from drifting buoys, near-surface measurements from Argo profiling floats, from the Global Tropical Moored Buoy Array (GTMBA) and from the Voluntary Observing System (VOS) climate Fleet (VOSClim). Each of these reference datasets has its pros and cons as shown in Figure 8.

Reference dataset	Pros and Cons
Ship-borne Radiometers	Traceable to SI; SST_{skin}; high accuracy; poor coverage
Drifting buoys	Uncertain calibration; near-global data; SST_{depth}; good coverage in recent decade
Argo near-surface	Near-global; acceptable sampling; very low uncertainty (calibration method to be analysed)
GTMBA	Good calibration; SST_{1m}; acceptable tropical and equatorial coverage (influenced by data collection);
VOS and VOSClim	Generally poor coverage; very high uncertainty on single sample

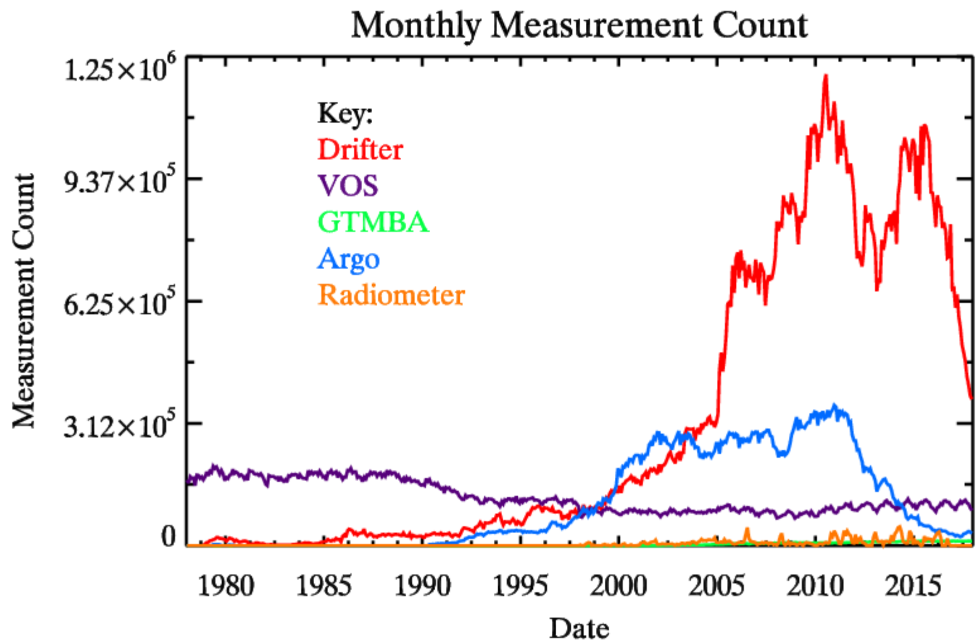

Figure 8: Pros and cons of the reference datasets and their monthly measurement count from 1980 to 2015. The radiometer, GTMBA sensors and Argo instruments are the most accurate but have the fewest surface measurements (although the coverage is good).

The biases and standard deviations calculated from a comparison of the datasets do not provide the uncertainty of each dataset individually, but are the sum of biases and combined uncertainty of a two dataset comparison. Additionally, the resulting statistics may be dominated by real changes in the SST that can occur within the predefined spatial and temporal limits.

Uncertainty modelling for Earth Observation (EO) relies heavily on understanding the instruments and retrieval processes, supporting error propagation by simulation and/or analytic techniques (Merchant and Embury, 2014). Indeed, validating satellite SST retrievals using reference data sets is not straight-forward and has many sources of error that cannot be easily corrected, but by considering each term we end up with a validation uncertainty budget (see equation 1). The metrological discipline of creating an uncertainty budget that is traceable (complete and defensible at each link the in the chain) can be used as a precedent for establishing the rigour and credibility of CDRs from EO (SST_CCI-URD-UKMO-201, Issue 2.1, 2017).The validation uncertainty budget can be represented thus:

$$\sigma_{Total} = \sqrt{\sigma_1^2 + \sigma_2^2 + \sigma_3^2 + \sigma_4^2 + \sigma_5^2} \quad (1)$$

Where (σ_1) is satellite uncertainty, σ_2 is reference uncertainty, σ_3 is temperature uncertainty resulting from spatial (surface) gradients, σ_4 is temperature uncertainty resulting from spatial (depth) gradients and σ_5 is temperature uncertainty resulting from temporal changes.

The magnitude of certain effects can be minimised using scientific knowledge of the variability in the upper ocean temperature, i.e. SST_{skin} should be retrieved from IR radiometers and the physics of the upper ocean used to compare to reference data at different depths. As the satellite uncertainty increases, the measurement of discrepancy also increases, which essentially means that both the uncertainty model and the validation of uncertainty model are right, i.e. they are self-consistent.

2. 4 Validation of Satellite SST Measurements

2.4.1 AATSR Validation

AATSR data was validated with ISAR data from 2004 until the loss of Envisat in April 2012, and it showed excellent consistency over the 8-year period. A total of 4149 match-up pairs were evaluated for a match-up window of +/- 2h of the overpass of AATSR and within 1 km of a confidently cloud-free pixel. The mean estimated difference compared to ISAR is -0.01 K for 1153 daytime match-ups (2 waveband retrievals) from 101 different overpasses, and 0.08 K for 2996 nighttime match-ups (3 waveband retrievals) from 138 overpasses. The Robust Standard Deviation (RSD) of the measurements is 0.25 K for day and 0.21 K for night data. Figure 9 shows the histograms for the AATSR-ISAR match-ups. The temperature range validated is from 5.3 °C to 24.2 °C.

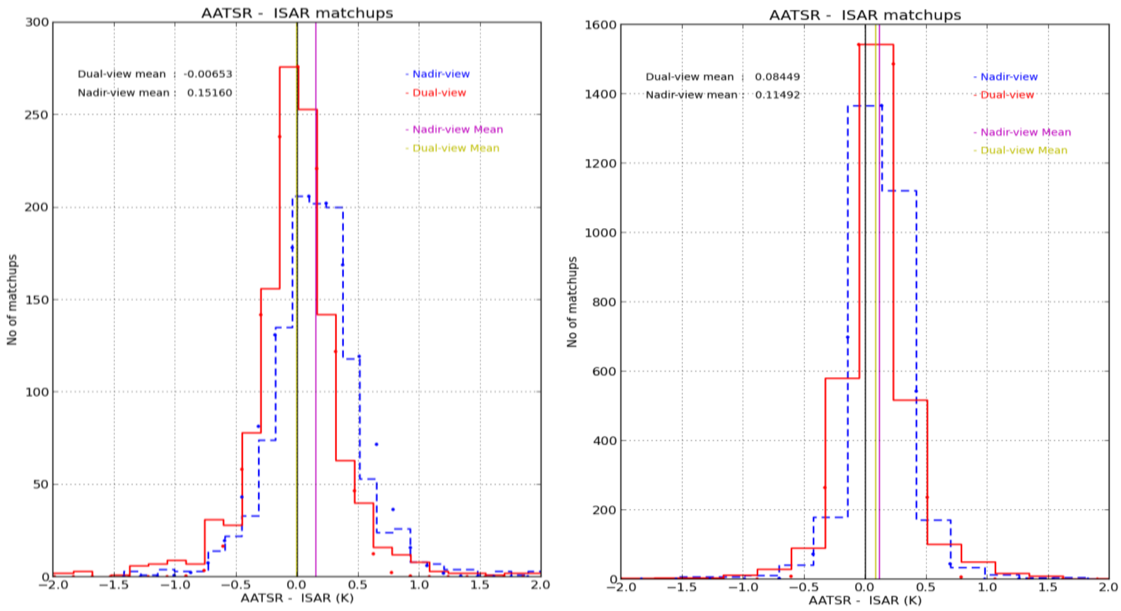

Figure 9: ISAR Histograms of Grade 2b match-up differences between AATSR and ISAR SST_{skin} records from deployments on the *Pride of Bilbao*, *Cap Finistére* and *Pont Aven* ships between July 2004 and April 2012, for night (left panel) and day (right). The solid red line shows the dual-view SST_{skin} product and the dashed blue line shows the nadir-only SST retrieval. The nadir-only match-ups have slightly different statistics than the dual-view match-ups with a difference between AATSR and ISAR of 0.11 K for nighttime data and 0.15 K for daytime data for a match-up window of ± 2h and 1km with an RSD of 0.22 K for the nighttime and 0.34 for the daytime.

Validation of long-term satellite data records requires the use of many different reference datasets. To this end, AATSR was also validated against other reference datasets on the ESA SST Climate Change Initiative (CCI) project, whose key aim was to provide a pixel level standard uncertainty for all products using independent measurements. Here, a range of reference measurements were combined with a skin/diurnal variability model (FKC; Fairall, Kantha and Clayson papers that describe models of the diurnal heating and skin layer effect) in order to adjust their depth and time to that of AATSR, see Figure 10.

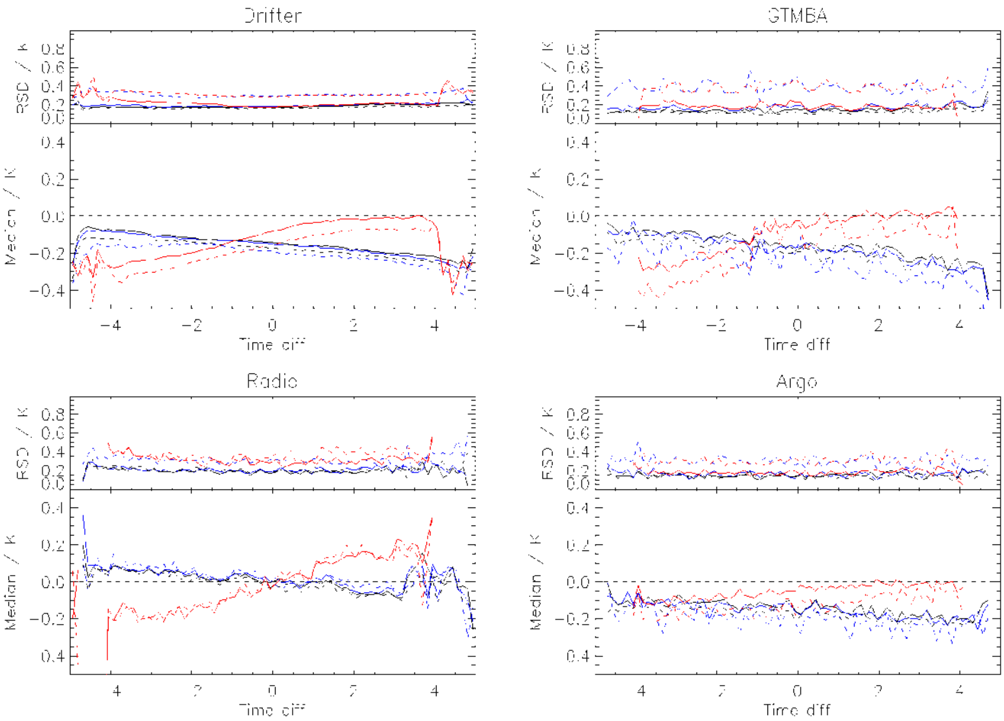

Figure 10: Adjusting for diurnal variability; the Radiometer skin data vs satellite data skin difference ('Radio' graph, bottom left) is zero, and the zero difference occurs when the satellite and shipboard radiometer measurements are closest in time. The blue traces indicate the ocean surface cooling during the night, and the red show the daytime heating. The drifters are sat at a 1m sea depth so the time difference between that and the satellite data skin should be approximately -1.7 seconds, which is what we see in the 'Drifter' graph. Again, this is in line with the physics and shows that the FKC adjustment results in good agreement between the reference datasets and the satellite data.

Overall, AATSR showed excellent performance over its lifetime when compared to ISAR data, exceeding its design specification of an accuracy of 0.3 K in the region of the English Channel and the Bay of Biscay.

2.4.2 SLSTR validation

SLSTR-A has been operational since July 2017, with an introduction of Bayesian cloud mask in April 2018, and reprocessed data is now available from April 2016 to April 2018 via the Copernicus Online Data Access (REProcessed) (CODArep). SLSTR-B data has been in production since June 2018 and an operational release is expected in March 2019.

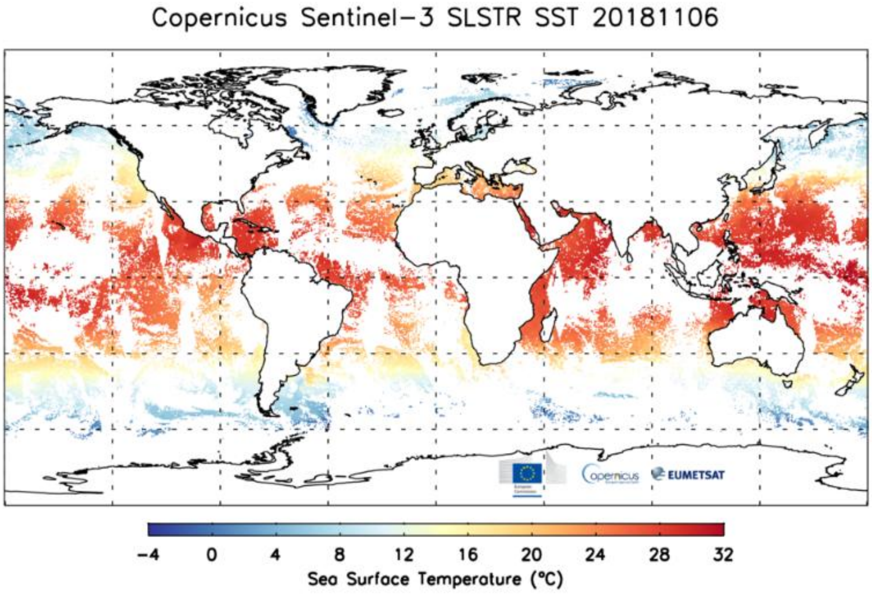

Figure 11: SST for Sentinel-3A and Sentinel-3B SLSTR (combined data) on 6 November 2018.

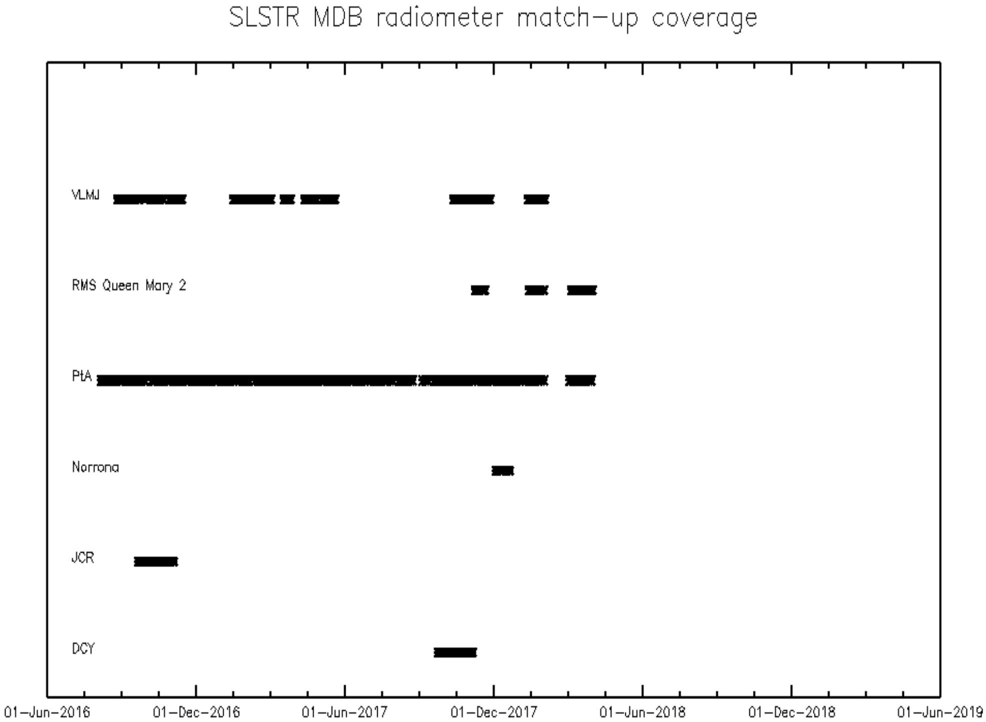

Figure 12: The current match-up database coverage of radiometer data for SLSTR, where PtA /Pont Aven deployment (ISAR), RMS Queen Mary 2 (SISTeR) and Norrona (ISAR) are deployments from the Ships4SST project.

SLSTR data was validated with ISAR and SISTeR data from August 2016 until March 2018. The validation of the SLSTR dataset shows good consistency over this period. The results for the Bay of

Biscay and English Channel operated by the UoS ISAR's on the Pont Aven are a mean difference of 0.01 K for 2475 day time match-ups and a mean difference of -0.02 K for 804 night time match-ups. The RSD for those match-up pairs are 0.27 K for the day time and 0.25 K for the night time. Figure 13 shows the histograms for the SLSTR-ISAR match-ups, with nighttime match-ups on the left and day-time match-ups on the right-hand side of the plot. The temperature range validated is from 0 °C to 35.4 °C.

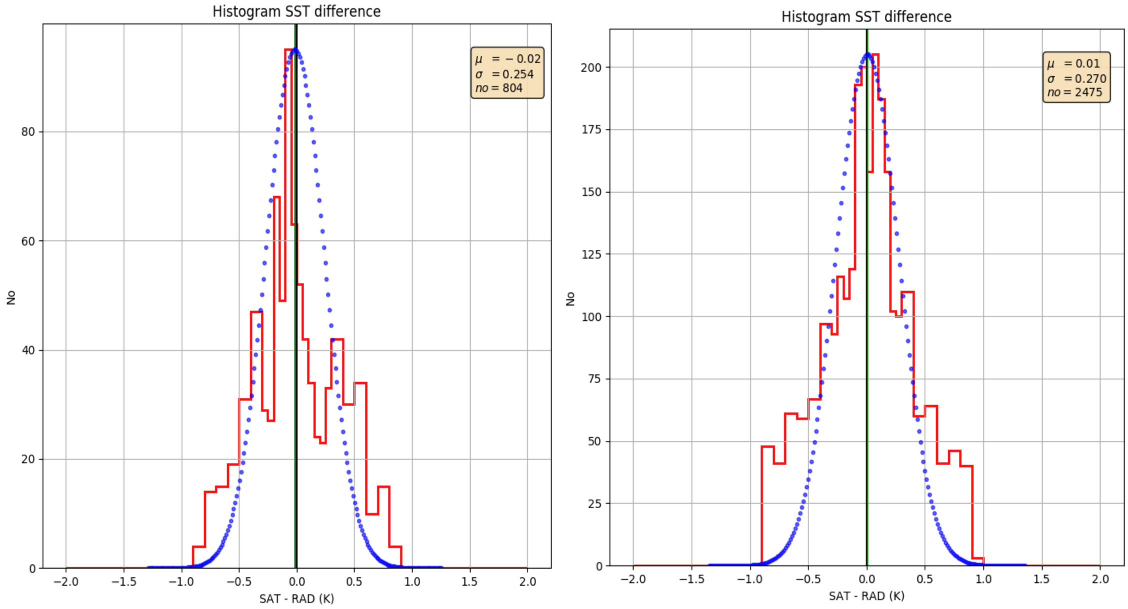

Figure 13: Histograms of Grade 2b match-up differences between SLSTR and ISAR SST_{skin} records on the *Pont Aven* between August 2016 and March 2018, for night (left panel) and day (right). The solid red line shows the SLSTR WST product and the dotted blue line shows a Gaussian fit to the data. The yellow boxes in the right hand top corners show the median (μ), the robust standard deviation (σ) and the number of matches (no) showing the SLSTR match-ups from the *Pont Aven* with a difference between SLSTR and ISAR of -0.02 K for nighttime data and 0.01 K for daytime data for a match-up window of ±2 hours and 1 km with an RSD of 0.25 K for the nighttime and 0.27 K for the daytime.

SLSTR has shown very good performance over the analysed three years when compared to ISAR and SISTeR data, exceeding its design specification of an accuracy of 0.3 K in the region of the English Channel and the Bay of Biscay and for night time SISTeR match-ups. Future validation work will include the implementation of AATSR match-up uncertainty methods on SLSTR validation. The initial tandem phase assessment of SLSTR-A and SLSTR-B Brightness Temperatures showed good agreement between the two instruments. There still seems to be some room for improvement in high latitude data and daytime global matches.

2.4.3 Linking AATSR and SLSTR, and AVHRR Harmonisation on SST CCI

The SST CCI project has constructed a ~35 year uncertainty-quantified SST climate data record, covering the period between 1983 and 2016 with the aim of making the time series independent from empirical tuning to other SST measurements and instead based on the physics of radiative transfer and instrument harmonisation. AVHRR harmonisation has been a particularly intensive task in the creation of a high stability, integrated long SST time series. It has involved the cross-calibration of AVHRR Brightness Temperature (BT) measurements with ATSR-2 and AATSR BTs and the referencing of SSTs to in situ instruments (pre 1995) and ATSR-2/AATSR/AVHRR (post 1995).

Due to the data gap between AATSR and SLSTR, and the high credibility of both as reference sensors, it is necessary to tie the sensors that fill the gap to both AATSR and SLSTR at either end and to make any adjustments necessary to account for bias. Metop-A is the key satellite chosen to do this as it carries AVHRR and IASI instruments that were operating at the same time as both AATSR and SLSTR (Merchant et al. 2019).

Notably, CCI+ will be the only programme internationally doing R&D on the long-term (35+ year) SST satellite record, since US Pathfinder (Kilpratrick et al., 2001, Casey et al., 2010) has ceased R&D and FIDUCEO will end in 2019.

2.4.4 MODIS and VIIRS Validation

The University of Miami has been using M-AERIs and ISARs to validate MODIS and VIIRS SST_{skin} retrievals. The M-AERIs now operate autonomously over satellite link and have been on long-term deployments on many cruises since 1996. The ISARs were first deployed on NYK ships in July 2005 but terminated in May 2018.

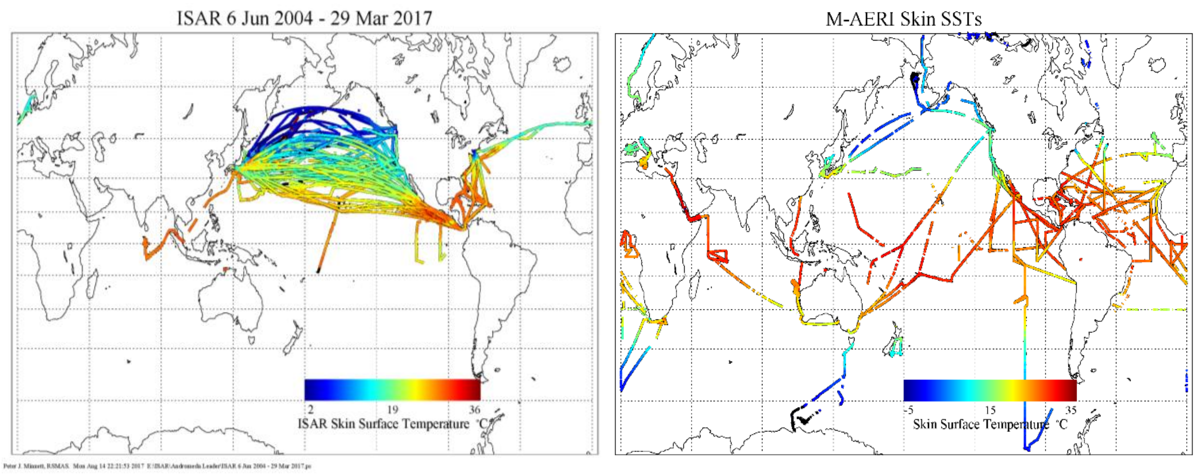

Figure 14: The SST_{skin} from ISAR cruises between 2004 and 2017 (left) and M-AERI SST_{skin} measurements between 8 September, 1998, and 10 June, 2017 (right). There are 194,597 data points on the M-AERI chart.

MAERIs and ISARs have been used for the validation against MODIS and VIIRS (see Table 1), and will be used for the SLSTRs. However, shipborne radiometers are not numerous and so to sample more of the parameter space that defines the accuracies of the satellite-derived SSTs, scientists have to rely on other sources too, such as drifting and moored buoys, and new technologies, such as Saildrones. A pilot project involving the University of Miami deployed a Saildrone off the west coast of America in 2018 for two months and other Saildrones will be deployed in the forthcoming NOPP MISST-3 (Multi-sensor Improved SST) project in the ice-free summer Arctic to provide data for improving SSTs from IR radiometers on satellites. It has been noted that although Saildrones have a simple IR radiometer, its absolute accuracy is questionable and the reflected sky radiance correction was not feasible during this cruise. Subsurface temperatures measured on the Saildrone have been shown to be useful for comparisons with satellite-derived SST (Gentemann et al., 2019).

Table 1: MODIS and VIIRS SSTs vs Shipborne Radiometers

MODIS Skin SST vs M-AERI and ISAR Skin SST. Temperatures in K					
Satellite and Algorithm	Mean	Median	Standard Deviation	Robust St. Deviation	Number
Terra SST Day	0.082	0.080	0.567	0.409	1025
Terra SST Night	0.048	0.034	0.467	0.337	2454
Terra SST4 Night	0.016	0.023	0.339	0.244	2467
Aqua SST Day	0.105	0.107	0.666	0.480	910
Aqua SST Night	0.020	0.027	0.489	0.353	1752
Aqua SST4 Night	-0.010	0.016	0.396	0.285	1858
VIIRS	0.030	0.009	0.196	0.142	81

2. 5 Software and Tools

2.5.1 Processing Ships4SST Data

Ships4SST data and match-up data are processed using Ifremer and Eumetsat tools. Data are automatically updated from the ingestion area where providers push their data and users can access the data at eftp.ifremer.fr (with login details). Up to 1700 ships4sst radiometer data measurements are received per month and data currently span over almost 10 years in the Felyx database. The data execution and flow can be seen in figure 15.

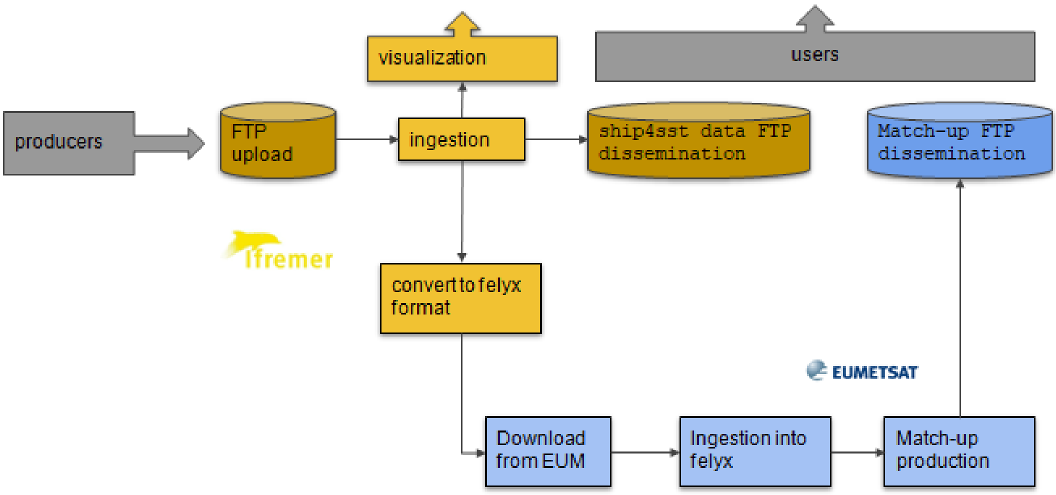

Figure 15: The data and execution flow of ships4sst data

Match-up production on Felyx involves systematic data subset extraction over predefined sites. Dynamic sites, that vary in latitude and longitude with time and which may be trajectories (buoys, cruises, hurricane), are used here, and a 400 x 400 (pixel) box is centred on the closest time trajectory location. SLSTR-ships4sst match-ups have been produced between August 2016 and March 2018 (as seen in section 2.4.2) and will be completed with full L2 and L1 data. Currently, there are ~1000 ships4sst matchups in total in Felyx, with more cruise data to be processed.

Data can be visualised using the ships4sst syntool, which shows the cruise location, track and SST_{skin} measurements (other parameters can also be added). Background SST_{skin} can also be shown on the world map. See figure 16 for an example screenshot.

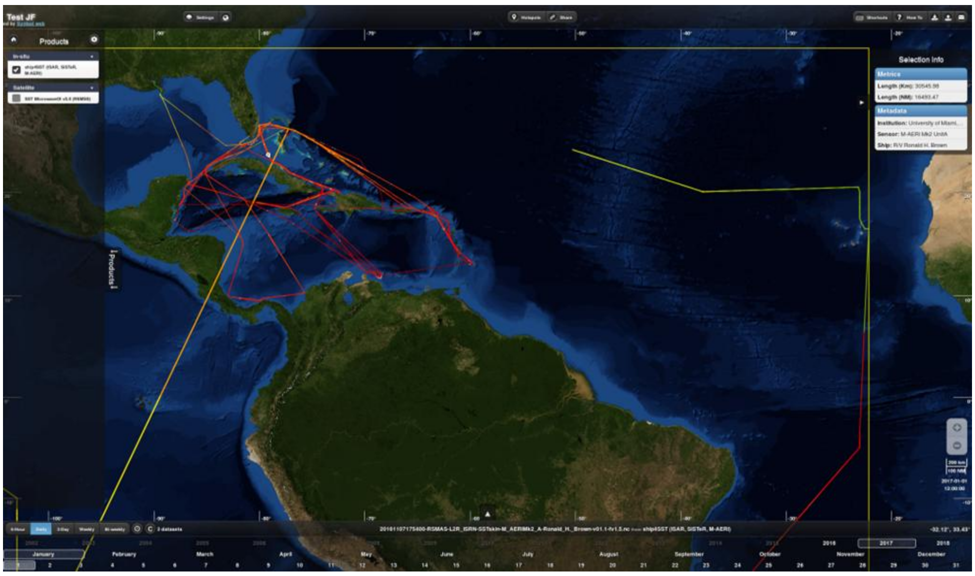

Figure 16: shows M-AERI data track around Central America on the 1st January 2017

2.5.2 The L2R Converter Tool

The L2R converter tool is used to produce the L2R format netcdf daily data files. It is user configurable and is an easy was to generate L2R by converting from ASCII. The tool is written in Python script (v2.7) and can be downloaded from the ISFRN FTP along with the user manual.

2.5.3 The KML Tool

The Keyhole Markup Language (KML) is used to describe and display geographic information. The tool is currently written in IDL although there are plans to port it to C or Python. The tool generates a KML file which is a text-based format containing elements that represent shapes, images, animations (etc.) and it can be used to generate ship tracks over Google Earth with details on date, time and SST_{skin} shown when you click on parts of the track (Figure 17). It is an obvious choice for displaying radiometer tracks over the ocean.

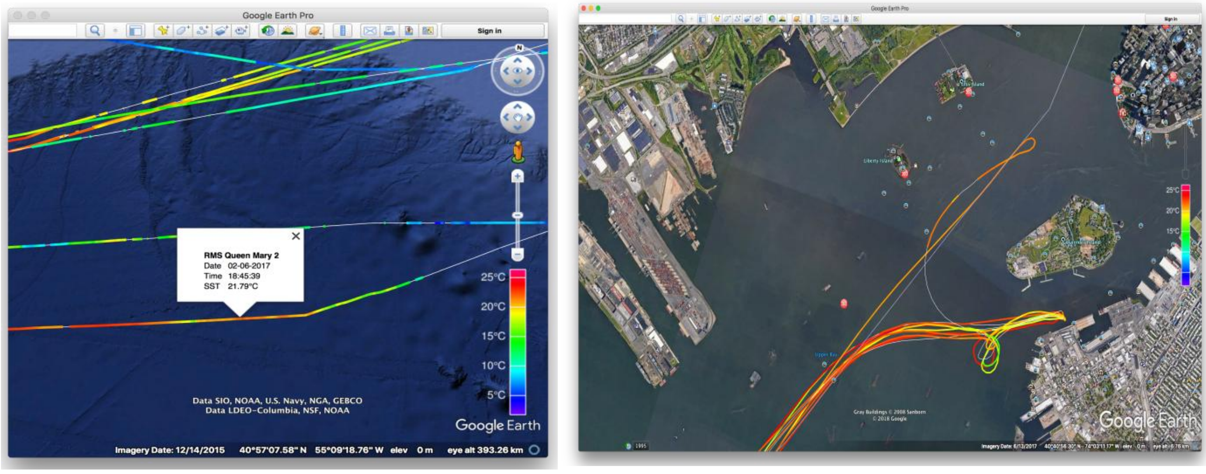

Figure 17: Users can retrieve impeded information by clicking on the track or view information from Google alongside the ship SST track.

3. Roadmap towards Future Measurements

Table 2 shows requirements and suggestions with strategies for implementation and comments. Each suggestion has been rated 1 to 5 for impact and difficulty and, if possible, a target date for implementation was given.

Table 2: Ships4sst service roadmap

Requirement / suggestion	**Strategies for implementation / Comments**	**Impact (5 high, 1 low)**	**Difficulty (5 high, 1 low)**	**Target Date**

Add more data and metadata to ISFRN database	Encourage more radiometer operators to join the network. New routes and reprocessing of existing data to L2R	5	being done routinely	ongoing
Improve information on observational methods	Write papers Publish more papers/reports/etc.	5	5 (because of time restraints)	April 2019
Ensure adequacy and continuity of the observing system	Performing more intercomparison exercises will help confirm the validity of uncertainty budgets, show the validity, equivalence and traceability of the measurements. This is difficult to do in the field as there is a geophysical component we do not necessarily know.	5	3 (have the knowhow, funding and time is limited)	2021
Improve openness and access to information	Increase the number of online documents on the Ships4sst webpage	5	2	2020
Quantified itemised uncertainties and sources of error in respect to SI	Source of errors might be tricky, and quantifying them, as if we can quantify them we correct for errors, otherwise they are uncertainties. Verification of uncertainty model (out at field).	5	5	ongoing
Push for more radiometers on ships of opportunities.	Radiometers can be more readily made traceable to SI than buoys Groups are starting to take up ISARS so this is increasing	5	N/A	ongoing
Develop new routes	The most important areas for new routes would be: 1. Reference ship tracks in frequently cloud free regions; this could be on a ship or fixed platform. This would fulfil the need for long-term consistency. 2. More radiometers going out into problem areas (arctic and islands) and the whole of the southern Ocean. 3. Aerosol regions, i.e. PIRATA North East Extension (PNE) mooring line at 24^{o}W or AEROSE (Nalli et al., 2011) – there are 6/7 cruises ready to go. Aerosols sometimes vary a lot so it is good to go to a few times.	4-5	2-3 (could use existing infrastruct ure)	Now
A database of information, including QA, on all radiometers to support validation	Documentation of processing versions, instrument maintenance etc. is available, but needs to be linked to reference sites, websites populated etc. A link from the ships4sst to QA3O information will be put online.	4-5	2-3	ongoing
Promotion of community protocols and best practises	Data submitted to the L2R archive should/must follow the ships4sst protocols.	4	2-4	ongoing

	Mandatory requirement to use L2R format. There may be some more work to do on protocols and metadata as protocols are followed within the ships4sst project (therefore easier) but not always used by everyone else. Is there evidence that people follow the protocols? The FRM4STS website needs to be linked to the ships4sst site.			
Measurements at a range of sea depths	We can only measure at the surface (skin), so should there be a range of oceanographic regimes, or do we want to include other sensors? Many ships already measure temperature at depth so they could be combined with SST_{skin}. Merge drifter data with Radiometer data for SI link Most ships are now measuring a range of data depths. A platform in the Mediterranean would be more useful than more measurements at different depths on ships because ships do not have FRM standards. Several months' worth of data of diurnal variability on various platforms would be useful.	N/A	5	2020
Sampling of coastal variability	Is already done, but we exclude most of the data for validation. Not necessarily an issue for climate studies. Interesting for high resolution missions. Large birds could be instrumented (e.g. on albatrosses and boobies feet) – Peter Minnett commented that the data was remarkably good when birds were used.	1	1	2020
Where would people like to see the focus of ships4sst.	Climate focus is important – i.e. service to operational validation of SST. Getting other members to contribute so that more data records could be included Develop, consolidate and maintain a network of radiometer operators to provide data of sufficient quality to allow optimal validation. Actively engaging with other operators Telecons with international partners/operators to get them more involved. A simplified next generation radiometer that could go on fixed platforms (might not need to be as robust as those on a vessel).	Various	Various	Various

The workshop discussions identified a number of areas to target that were both High Impact and Low Difficulty, leading to a high likelihood that these suggestions will come to fruition in the near future. One of these is the need to improve openness and access to information. Strategies for implementing this included increasing the number of online documents on the ships4sst webpage, and phase 2 (called FRM4SST) of this project is the prime time to do this. The ESA-funded FRM4SST project started in May 2019 with the objective of continuing and expanding on the work done in the ships4sst contract. Linking the ships4sst project website to relevant sources of information was suggested several times. Whilst there are already a number of links online, it is clear that more links with more information and details are required. Again, this will be addressed in the FRM4SST project.

One of the highest priority areas was to increase the understanding of and improving the uncertainties associated with radiometer SST_{skin} measurements. There were several suggestions for this; for example, performing intercomparison exercises help to confirm the validity of uncertainty measurements on radiometers. Past intercomparison exercises have proved successful and with funding, time and international cooperation, future intercomparison exercises could be performed. Whilst there are geophysical factors that can make improving uncertainties in field measurements tricky, the need for increased time and funding to perform the intercomparison experiments and analyse the data seems to be the main factor increasing the difficulty level of uncertainty-related requirements to the highest rating of 5.

When specifically asked where participants would like the project to focus on, there were a number of suggestions including:

- Focussing on the validation of SST is important for climate studies.
- Consolidating the network and encouraging new members to contribute data and information by actively engaging with other radiometer operators.
- Maintain a network to provide data of sufficient quality to allow optimal validation.
- Looking into creating a cheaper, simplified radiometer that can go on fixed platforms. It need not be as robust as an instrument on a vessel but there could be opportunities to deploy more fixed instruments.

Plans to promote the ISFRN and actively engage with the community will continue into the FRM4SST study funded by ESA, which continues the work of the Ships4SST project.

4. Conclusion

There is a clear need for shipborne radiometer deployments, whether for gap bridging between satellite deployments or for the referencing and validation of satellite SST_{skin} retrievals to FRM standards. The long time period of radiometer deployments has resulted in greater understanding of radiometer instrumentation, so that now radiometers are autonomous and robust enough to work in most environments. Online monitoring and real time transmission of measurements can also be set up to ensure that data are available in near real-time and problems with the instrument become apparent immediately, enabling the operator to take appropriate action, which may be to alert someone onboard to check the instrument and return it to operations whilst a ship is out at sea.

ISAR deployments have not been limited to SST_{skin} data collections via cruises or side-by-side intercomparisons, there have been a number of scientific campaigns over the years over ice and land. For example, a field campaign was implemented in 2016 using 3 research teams and 6 TIR radiometers mounted on sea ice. Experiments included intercomparisons, spatial variability and angular emissivity (J. L. Hoyer et al. Field Report, 2017). The successful campaign also highlighted the fact that there is currently no all year round radiometric observation of Ice Surface Temperature (IST). The provision of FRM TIR for IST measurements is an avenue that radiometer operators would like to explore in the future, as well as the possibility of bringing in more ships of opportunity to expand the network of in situ SST radiometers.

Work done by those deploying shipboard radiometers has resulted in the establishment of protocols, best practices and a recommended data format that is now used by three instruments types (the ISAR, M-AERI and SISTeR). As shipborne radiometers provide a traceability route for satellite SST_{skin} retrievals they are therefore a pathway to generating CDRs from satellite SST measurements. The ISFRN has helped to develop and take these practices forward. The network is also interested in historical records. Further international collaboration is expected with Korea now that ISAR training has taken place, and with South Africa regarding instrument loan.

Radiometers provide an essential source of data for satellite SST_{skin} validation and for FKC adjustments (at skin surface depths), although the resulting statistics are generally noisier than for other primary in situ type due to the reduced number and consequential distribution of shipborne radiometers. Current results show that more work needs to be done on clarifying the uncertainties. This will require more match-up data between satellites and in situ, which are expected to become available as SLSTR data from two instruments and 19 ISARs keep contributing data. Comparisons against similar radiometers and against other in situ SST measurements are also key to ensuring the robustness of the instruments and to verify the validity of the data they provide.

The almost 10 years worth of radiometer data and match-ups on the Felyx database, combined with the visualisation tools, enable users to easily visualise SST_{skin} radiometer data. If a user is so inclined, they can find and visualise the SST_{skin} measured by the ISARs, MAERI and SISTeR at any point along a ships track, as well as a number of other parameters.

The ISFRN Workshop brought together a number of experts in the radiometry field to present and discuss the latest results in shipborne radiometry and satellite SST validation activities, as well as to look ahead to the future of shipborne SST radiometry. Whilst this paper has only summarised the key information from the workshop presentations and discussions, it is clear that shipborne radiometry is gaining strength and recognition for the consistency, stability and usefulness of its measurements in validating satellite data from instruments including AATSR and SLSTR. The ISFRN has gained support from the radiometer community and acquired new data with the intention to expand further, creating a universal data centre that provides easier access to shipborne SST radiometer data that are both accurate and consistent in format and quality.

The presentations, protocols, procedures and reports are all available on the Ships4sst website at www.ships4sst.org/documents.

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