Sea Surface Temperature in Global Analyses: Gains from the Copernicus Imaging Microwave Radiometer

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Sea surface temperature in global analyses: gains from the Copernicus Imaging Microwave Radiometer

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Abstract: Sea surface temperatures (SSTs) derived from passive microwave (PMW) observations benefit global ocean and SST analyses because of their near-all-weather availability. Present PMW SSTs have real aperture-limited spatial resolution in excess of 50 km, limiting the spatial fidelity with which SST features, reflecting ocean dynamics, can be captured. This contrasts with the target resolution of global analyses of 5 to 10 km. The Copernicus Imaging Microwave Radiometer (CIMR) is a mission concept under consideration as a high-priority candidate mission for expansion of the Copernicus space programme. This instrument would be capable of real aperture resolution <15 km with low total uncertainties in the range 0.4-0.8K for channels between 1.4 and 36.5 GHz and a dual-view arrangement that further reduces noise. This paper provides a comparative study of SST uncertainty and feature resolution with and without the availability of CIMR in the future SST-observing satellite constellation, based on a detailed simulation of CIMR plus infra-red observations and the processing of global SST analyses with 0.05° final grid resolution. Simulations of CIMR data including structured errors were added to an observing system consisting of the Sea and Land Surface Radiometer (SLSTR) on Sentinel-3A and the Advanced Very High Resolution Radiometer (AVHRR) on MetOp-A. This resulted in a large improvement in the global RMSE for SST from 0.37K to 0.21K for January and 0.34K to 0.23K for July. There was a particularly noticeable improvement in the performance of the analysis, as measured by the reduction in RMSE, for dynamical and persistently cloudy areas. Of these, the Aghulas current showed an improvement of 43% in January and 48% in July, the Gulf Stream 70% and 44%, and the Maritime Continent 50% and 40%.

Keywords: passive microwave; sea surface temperature; CIMR; OSTIA;

1. Introduction

Measurement of sea surface temperature (SST) is crucial to the understanding and prediction of the atmosphere and ocean. SST regulates the exchange of moisture and heat [1,2] between the two and thus controls the thermal structure of the upper ocean and sets the boundary conditions needed for numerical weather prediction. Errors in SST can lead directly to a decrease in NWP skill [3]. SSTs retrieved from infrared (IR) sensor data generally have superior spatial resolution (~1 km) and retrieval accuracy (0.2 to 0.4 K) to passive microwave (PMW) sensors (~50 km and 0.35 to 0.5 K for recent and current missions) [4-7]. However, they are limited to cloud-free regions whereas PMW sensors are able to make measurements through cloud. This greatly increases their coverage and makes them particularly important for regions of persistent cloud such as the high-latitudes in winter.

The Copernicus Imaging Microwave Radiometer (CIMR) is a mission concept under consideration as a high-priority candidate mission for expansion of the Copernicus space programme (the Sentinels). The concept includes deployment of a ~7 m mesh antenna capable of real aperture resolution <15 km at 6.9 GHz (required for cool-water SST estimation). The CIMR mission is motivated by the EU Arctic policy [8], whereby monitoring of the physical properties of the changing high-latitude environment is essential for sustainability, economic development and environmental protection. Its primary objectives are the retrieval of sea ice concentration (SIC) and SST. The requirement for SIC is for spatial resolution ≤5 km with a total standard uncertainty of ≤5% and for SST is spatial resolution ≤15 km with a total standard uncertainty of ≤0.2 ±0.1 K[9]. The CIMR mission will deliver both high-latitude and global data with near-global coverage every day. CIMR SSTs will therefore improve the observability of ocean dynamics reflected in SST compared to an infra-red-only SST dataset, particularly in areas of persistent cloud: the Arctic, Southern Ocean, north Pacific and Atlantic oceans, marine stratiform regions, and the inter-tropical convergence zone including the tropical warm pool. The targets for the uncertainty components are given in Table 1. Measurements from both the forward and rearward arcs of CIMR's conical scan will be available, enabling averaging of retrievals to reduce noise. This combination of features implies that CIMR SSTs are expected to have simultaneously higher spatial resolution and lower noise uncertainty than present PMW SSTs [9].

Table 1 Uncertainty components for each of the CIMR channels. The columns give the total uncertainty as well as the radiometric, orbital stability, lifetime-stability and pre-launch calibration contributions to the total uncertainty budget.

Channel (GHz)	U_{total}	$U_{\text{NE}\Delta\text{T}}$	$U_{\text{orb-stab}}$	$U_{\text{life-stab}}$	$U_{\text{pl-cal}}$
1.41	0.5	0.3	0.2	0.2	0.2
6.9	0.4	0.2	0.1	0.2	0.2
10.65	0.45	0.3	0.1	0.2	0.2
18.7	0.6	0.4	0.2	0.2	0.2
36.5	0.8	0.7	0.2	0.2	0.2

The aim of this study is to examine the effect on SST analyses of adding CIMR to the IR-observing constellation, here represented by the Advanced very-high-resolution radiometer (AVHRR) instrument on-board Met-Op A and by the Sea and Land Surface Temperature Radiometer (SLSTR) carried by Sentinel-3A. Synthesised observations were provided as input to the Operational Sea Surface Temperature and Sea Ice Analysis system (OSTIA) [10] in different combinations as set out below.

The OSTIA system is in operational near-real time use by the Met Office. It operates by ingesting satellite and in situ SSTs and optimally combining them to produce estimates of daily, global, foundation SST (defined as SST free of diurnal variability[11,12]). A climate configuration of the system generates SST analyses from satellite data only, which are representative of the daily average at 20 cm depth [7] and this is used in this study. For each day, the system generates a background field based on the persistence of the previous day's analysis, with a weak relaxation to climatology. For the open ocean, the relaxation timescale is 30 days. The background is combined with the satellite SSTs with relative weights determined by their uncertainties. A background error covariance matrix is specified *a priori* based on two components, one representing errors due to mesoscale ocean features and one capturing larger scale errors such a synoptic weather systems. The uncertainty associated with each retrieved SST is used with errors assumed to be uncorrelated. The new analysis is then calculated using the NEMOVAR system[13] to minimize the cost function

$$\mathrm{f} = \delta x^{\mathrm{T}} \mathbf{B}^{-1} \delta x + \delta y^{\mathrm{T}} \mathbf{R}^{-1} \delta y \quad (1)$$

where δx is the difference between the new analysis field and the background state, $\boldsymbol{B}$ is the background error covariance matrix, δy is the difference between the newly-measured SSTs and those in the background state and $\boldsymbol{R}$ is the observation error covariance matrix[14].

2. Methods

To understand the impact of CIMR the future observability of SST, we have undertaken a simulation study that provides synthetic observations to the OSTIA system. By providing input data with and without CIMR observations and with and without realistic observational errors, we can test the effect of the increased coverage provided by adding CIMR data to the IR constellation and whether this effect remains when allowance is made for the increased uncertainties associated with PMW-derived SSTs. To achieve this, a "truth" dataset was required from which simulated observations for CIMR, SLSTR and AVHRR could subsequently be derived and to which analysis fields could be compared. To act as SST truth, we obtained data generated as part of the North Atlantic Climate System Integrated Study (ACSIS) [15], consisting of the output of a free-running coupled general-circulation simulation using the Nucleus for European Modelling of the Ocean (NEMO) model [16]**.** These data were provided on the tripolar, curvilinear, ORCA12 grid[17,18], with approximate 1/12° resolution, and regridded here to an equiangular 0.05° grid for input to OSTIA. As the ORCA grid is slightly coarser than the target OSTIA grid, there is the potential for loss of feature resolution at the smallest scales. Consequently, sharpening was applied, using a 2-D Laplacian filter, to increase the power at shorter length scales to match the -11/3 power law expected for sea surface height and SST in the open ocean [19-21].

In order to simulate IR observations of the "truth" dataset with appropriate spatial coverage, it was necessary to apply realistic masking to the data. The largest single cause of invalid IR-based SST values over the ocean, within the satellite swath, is the presence of cloud. Suitable masking was achieved using L3U data for the two IR instruments from 2018 generated with the processor (GBCS) used for the Sea Surface Temperature Climate Change Initiative project [7,22-24] and the Copernicus Climate Change Service Climate Data Store [25,26]. L3U data were generated at 0.05 resolution with multiple files a day, each corresponding to an input L1 file. The SST in each L3U file was replaced with the value from the "truth" dataset for that day of the year at all locations with a valid SST value and with a quality level of 4 or higher. In January, this results in 14.0±0.6% of global ocean cells having at least one AVHRR observation on a given day and 12.4±0.5% having at least one SLSTR observation. Being based on a free-running model, the choice of year for the "truth" data was arbitrary rather than specifically 2018. Model cells with SST less than -1.7°C were interpreted as the locations of sea ice. The resulting dataset constituted the SSTs that would be derived in the case of a perfect observing and retrieval system for the two infrared instruments, given the cloud distribution of the target days.

To provide a more realistic observational dataset, synthetic noise was added to the SST in the "perfect" files based on the uncertainty terms provided for each cell in the L3U files. These are (with typically values for AVHRR) large-scale correlated uncertainty (~0.1 K), adjustment uncertainty (0.05-0.1 K), synoptically correlated uncertainty (0.1-1.0 K) and uncorrelated uncertainty (0.05-0.2 K). Large-scale correlated uncertainties are those that arise from effects that can be assumed to be correlated everywhere and over long time scales (such as calibration of the satellite sensor). The adjustment uncertainty arises from the process of adjusting SSTs to a standard time and depth. The synoptically correlated uncertainty arises from correlations in the atmospheric conditions between SST retrievals. Both the adjustment and synoptic uncertainties are assumed to be correlated over 100 km for IR sensors and 1 day. Uncorrelated uncertainties arise from effects that are not correlated from location to location such as random noise in the satellite sensors [27,28]. Each of these contributions was considered in turn and, for each, a value was added to the SST in each cell in the perfect dataset of with an appropriate magnitude and correlation properties.

A single large-scale noise value was applied to all cells in a given L3U file by selecting a random number from the Gaussian distribution with a standard deviation given by the mean of the large-scale correlated uncertainty values in the corresponding file. Noise values corresponding to the adjustment and synoptically correlated uncertainties were generated using a common method. Here

a value was chosen at random for each cell on a 1° resolution grid from a Gaussian distribution with a standard deviation given by the mean of these uncertainties over all of the 0.05° resolution cells falling within the 1° cell. These values were then interpolated back down to 0.05° resolution to give a noise value to add to each cell of an appropriate size, that varied smoothly and had correlations over the correct lengthscale (~100 km) for synoptic weather systems. The uncorrelated uncertainty values for each cell were used directly by choosing a random number chosen from a Gaussian distribution with the given standard deviation.

Representative daily L3C CIMR data were also generated based on the model "truth" dataset. An initial sea ice mask was applied on the same basis as for the IR data. The edges of the mask were extended by two additional cells in both latitude and longitude to represent the need to avoid side-lobe contamination when measuring SST. A median filter was subsequently applied over a 3x3 box to obtain a SST value as seen by an instrument with a 15 km footprint. These data were then subset to every third pixel in each direction to ensure the independence of each cell being fed to the OSTIA system and a mask was applied to eliminate cells within 25 km of land. Finally, a mask was applied based on the daily coverage expected for the instrument. Analogously to the IR instruments, the resulting data represents the SSTs that would be derived in the case of a perfect observing and retrieval system for CIMR.

To ensure the correct weighting of the CIMR observations by the OSTIA system and in order to generate appropriate synthetic observational noise, values were derived for the same 4 uncertainty terms considered for the IR data. The uncorrelated uncertainties were taken from [29] that looked at the result of the instrumental NeΔT on the expected retrieval uncertainty of SST from CIMR. The dependence of this uncertainty on SST was retained but, in the absence of specific meteorological information, it was calculated using fixed values of wind speed (7 m s^{-1}), salinity (35 psu) and total column water vapour (14 kg m^{-2}). A similar analysis to [29] that tested the effect of the orbital instability (rather than radiometric) uncertainty on retrieved SST was used to derive values for the synoptically correlated uncertainty of SST. A value of 0.1 K for the adjustment uncertainty was assumed and the large-scale uncertainty term was set to 0 on the assumption of a well-designed and calibrated retrieval scheme that removed orbit-to-orbit biases. An assumption was made that uncertainties were independent across orbits and thus reduced by $\sqrt{N_{obs}}$ for cells with multiple observations on a given day. Noise values were derived from these terms for each cell using the same prescription as for the IR data with the exception that the synoptically correlated uncertainties were derived using a 10°-resolution grid rather than 1°-resolution grid. This ensured a correlation lengthscale of ~1000 km appropriate to the variability in the orbital stability which was assumed to be the dominant effect for this term. An example global SST and the added noise field for CIMR are shown in **Erreur ! Source du renvoi introuvable.**.

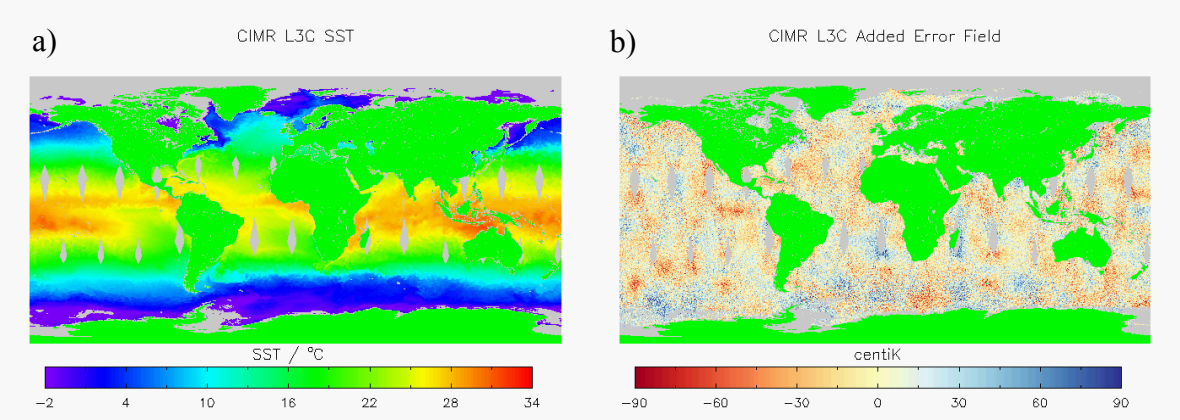

Figure 1 a) Example of the daily SST field from a CIMR L3C file; b) the added error field for this CIMR L3C field

The above datasets were used as input to the OSTIA system in four configurations: "perfect" IR-only, "perfect" combined IR and CIMR, IR-only with realistic errors, and combined IR and CIMR with realistic errors. SST analysis fields were generated for January and July for each configuration. In each case, the first two weeks of the analysis were discarded as a spin-up period and the rest of the month used for assessing the error characteristics of the analysis outputs for each configuration. The data processing methods are summarized in Figure 2 and Figure 3.

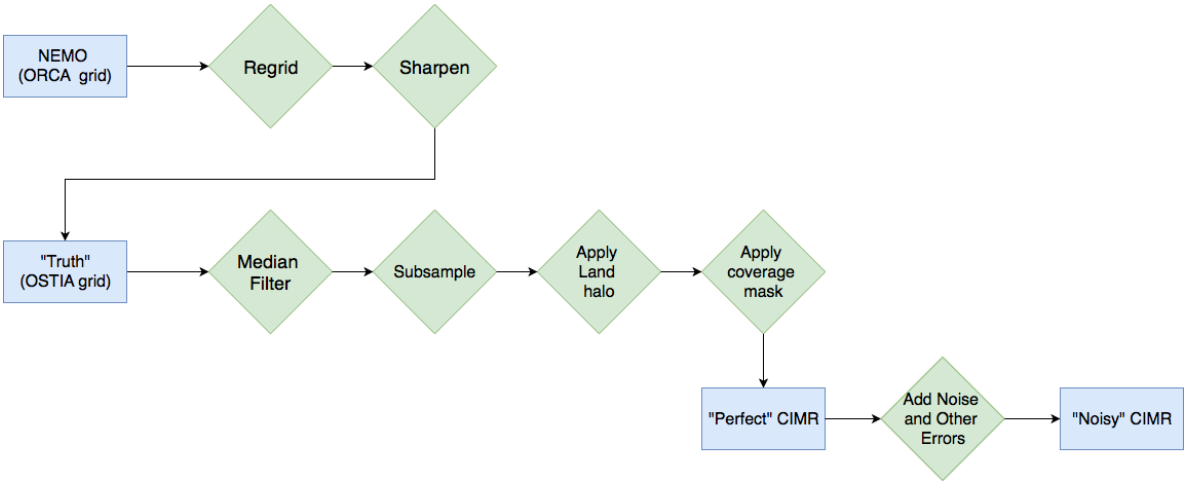

Figure 2 Processing steps involved in generating the synthetic CIMR data

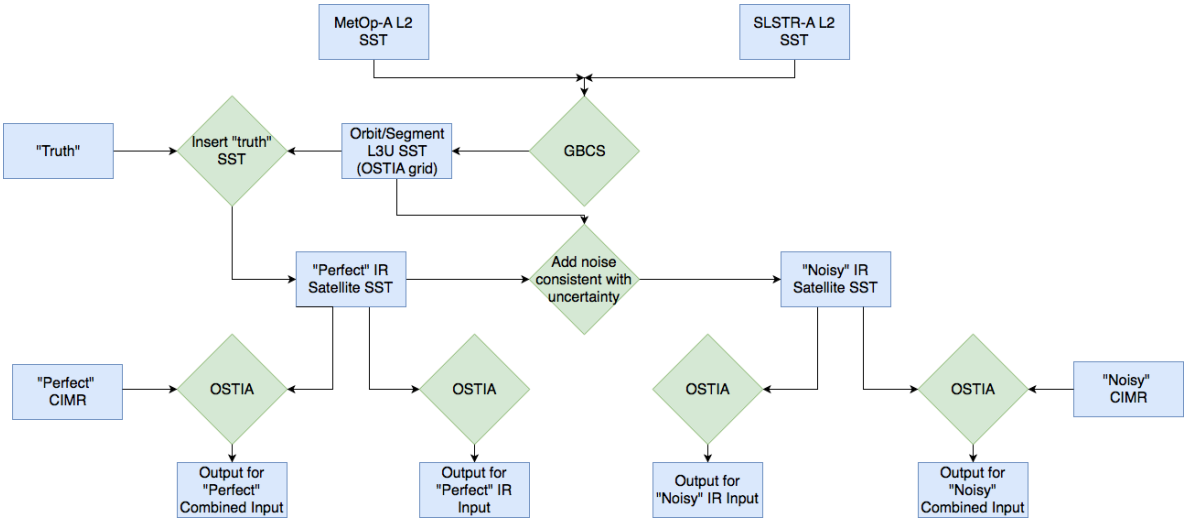

Figure 3 Processing steps involved in creating synthetic SST data for AVHRR and SLSTR

3. Results

3.1. Error Statistics

The mean and standard deviation of the error in the daily analysis SST were formed by comparison with the original "truth" dataset for the day. Histograms of the distribution and global maps of these statistics are shown for January in Figure 4 and Figure 5 respectively for the perfect input data cases. Similar comparisons using input data with realistic errors are shown in Figure 6 and Figure 7. The change in the root-mean-square error (RMSE) resulting from the addition of the CIMR data to the analysis inputs is shown in Figure 8. Results for July are similar to those for January and so just the maps of the errors statistics are shown for the data with realistic errors and the change in RMSE in Figure 9 and Figure 10.

Both Figure 4 and Figure 6 show a clear improvement in the error distributions with the addition of CIMR data and imply an improved ability of the analyses to reproduce the "truth" dataset. As might be expected, the OSTIA analyses in Figure 5, Figure 7 and Figure 9 show patches of larger error standard deviations in regions of dynamical SST such as around the Aghulas current and the Gulf Stream. More widely, for the infrared-only reconstructions, the error standard deviations appear larger in the southern hemisphere in January and the northern hemisphere in July. This is counter-intuitive one might expect summer to result in decreased cloudiness and thus improved coverage. In January, for the southern hemisphere AVHRR and SLSTR have 16.1±0.9% and 14.5±0.9% daily hemisphere coverage respectively compared to 11.5±0.8% and 10.1±0.5% for the northern hemisphere. However, in July, there is a more mixed coverage picture: 13.0±1.1% and 12.0±0.8% coverage for the southern hemisphere compared to 10.8±1.1% and 12.5±1.1% for the northern hemisphere. This implies that rather than coverage, the differences in performance between the hemispheres is due to increased variability in summer.

The differences between northern and southern hemispheres become less pronounced with the addition of the CIMR data. There are still patches of larger RMSE in the dynamical areas even though Figure 8 and Figure 10 show that the biggest improvements from the addition of CIMR data are in these regions. The north-west Pacific in July appears to remain a difficult region to reconstruct. Close examination shows that the coastal areas have larger RMSE than the open ocean in all the analyses.

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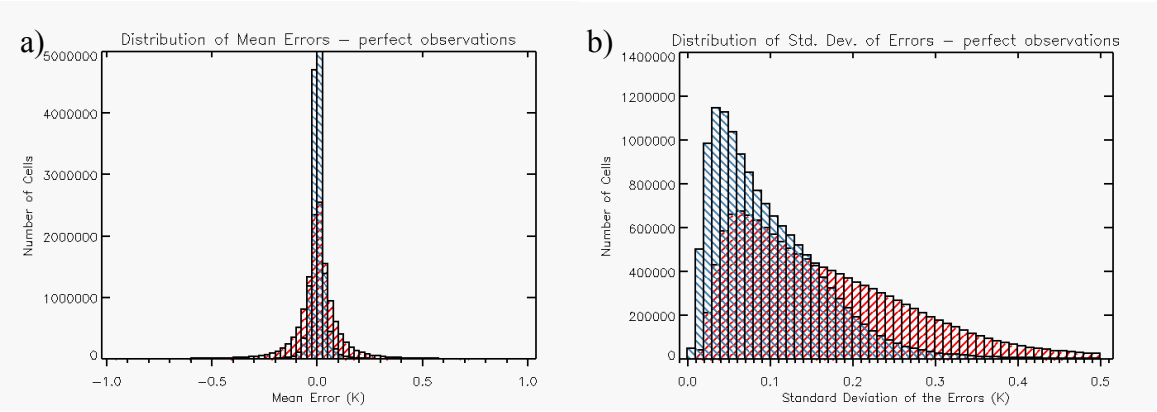

Figure 4 Statistics of the differences between January analysis SST fields and original "truth" SST IR-only (red) and combined IR and MW (blue) input data: (a) Mean error for perfect input; (b) Standard deviation of the error for perfect input.

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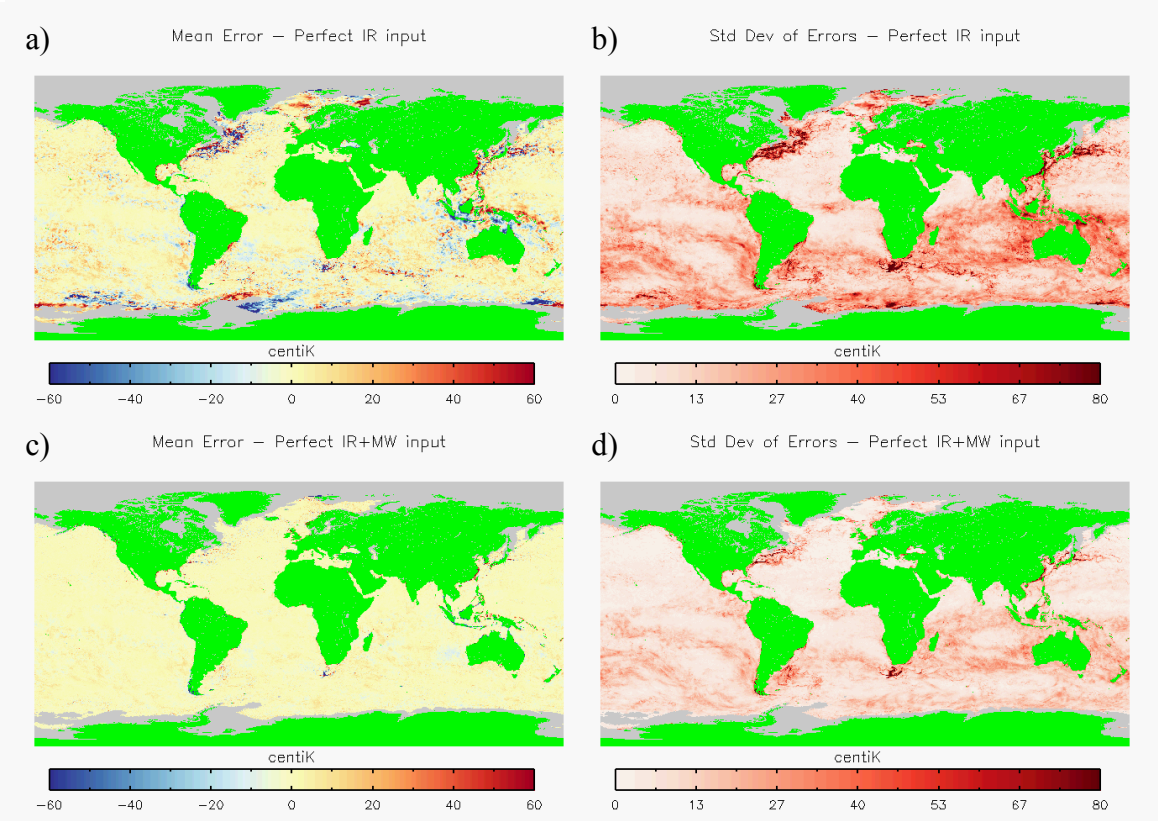

Figure 5 Maps of the January error statistics: a) Mean Error - perfect IR data only; b) Standard deviation of the error - perfect IR data only; c) Mean error - combined perfect IR and CIMR data; d) Standard deviation of the error - combined perfect IR and CIMR data.

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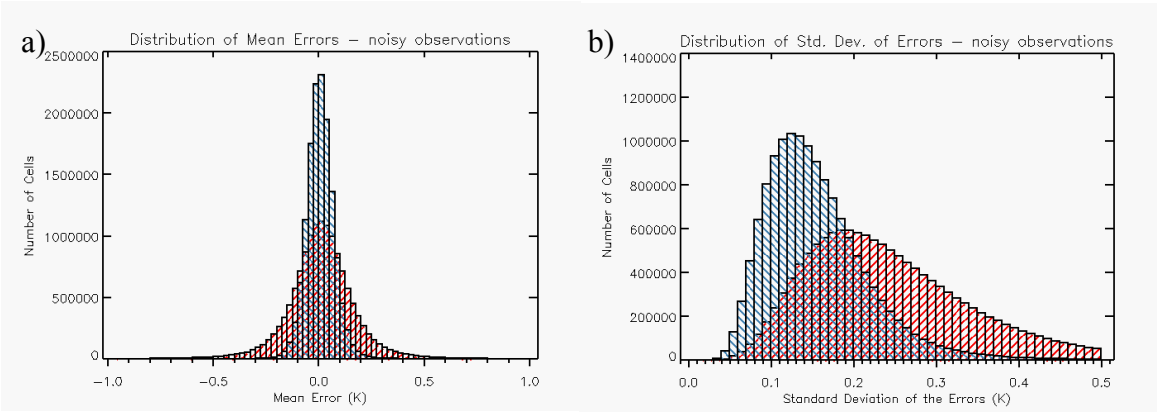

Figure 6 Statistics of the differences between January analysis SST fields and original "truth" SST for IR-only (red) and combined IR and MW (blue) input data with realistic errors: (a) Mean error (b) Standard deviation of the error.

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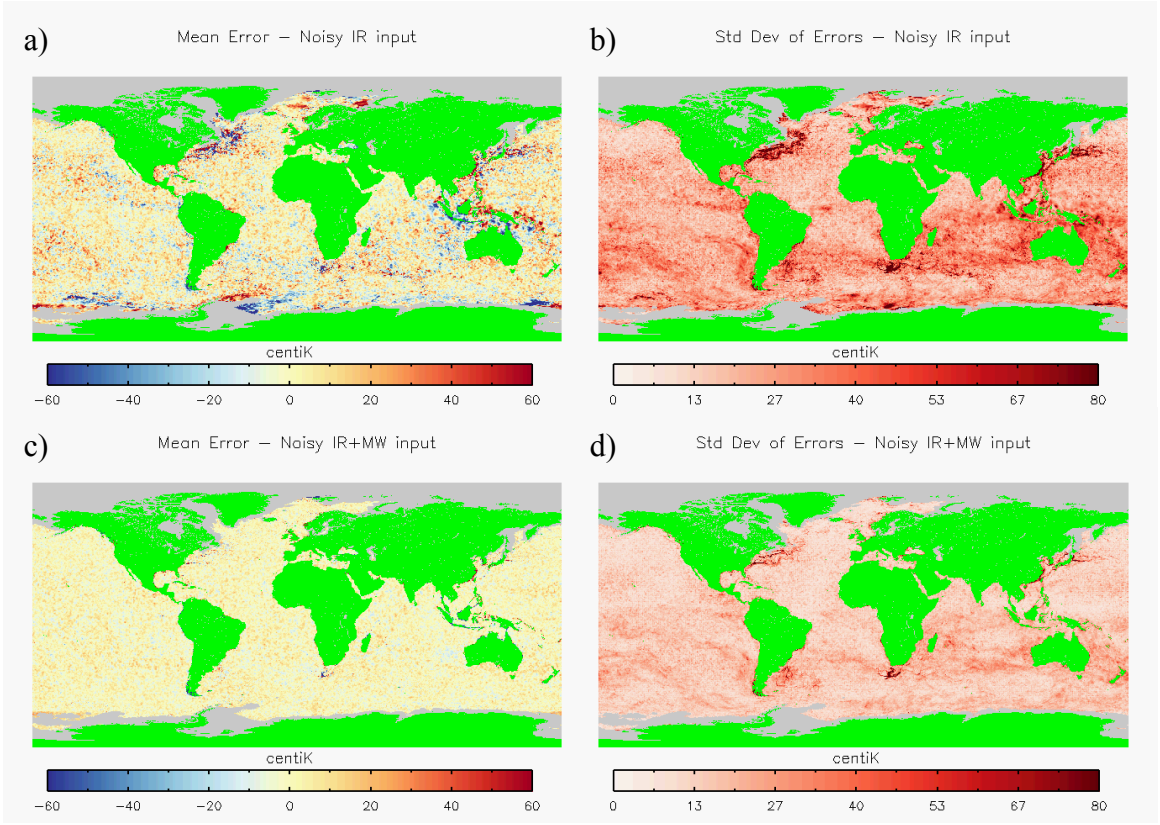

Figure 7 Maps of the error statistics during January for input data with realistic errors: a) Mean Error - IR data only; b) Standard deviation of the error - IR data only; c) Mean error - combined IR and CIMR data; d) Standard deviation of the error - combined IR and CIMR data.

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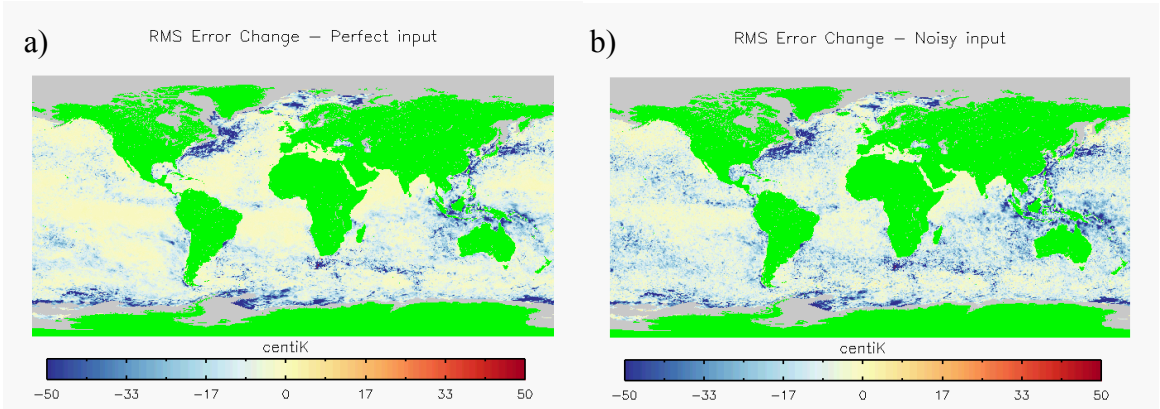

Figure 8 Change in the RMS error of the reconstructed SST field in January from adding CIMR data to the input for: (**a**) perfect input data; (**b**) input data containing realistic errors.

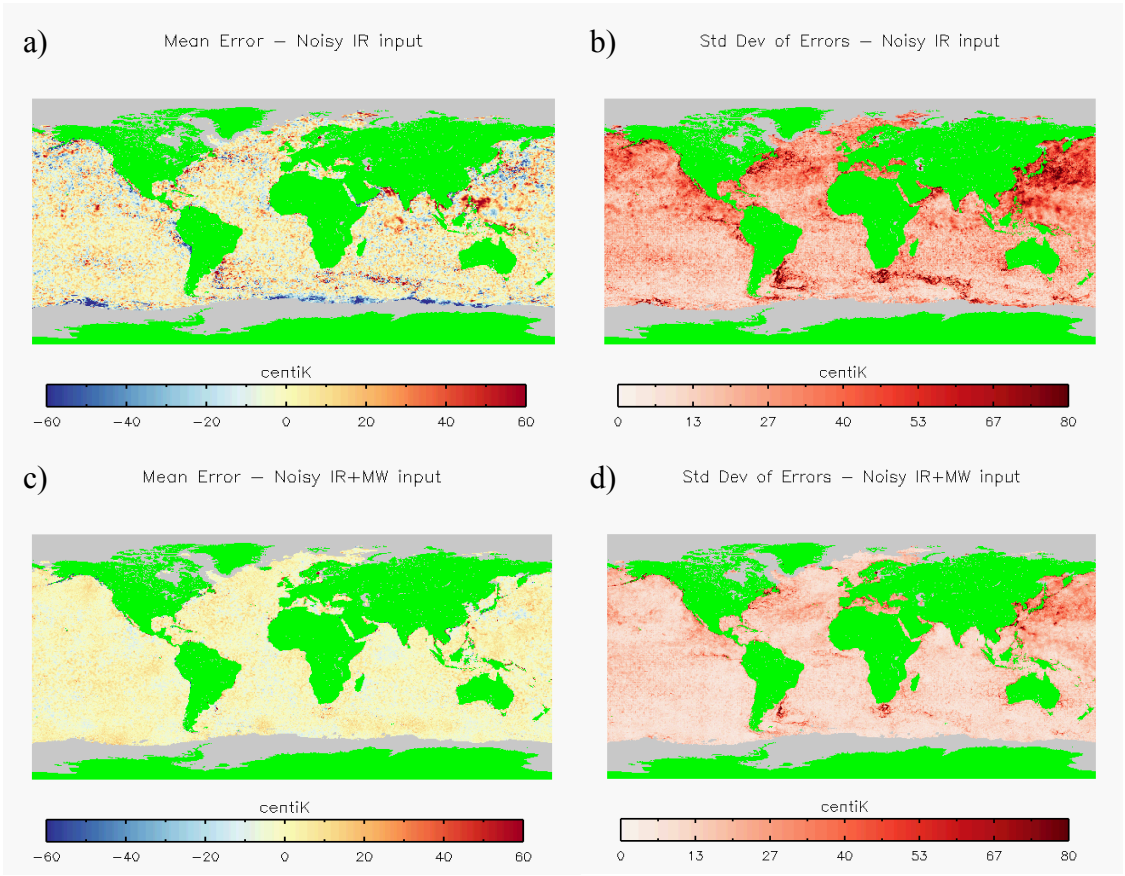

Figure 9 Maps of the error statistics during July for input data with realist errors: a) Mean Error - IR data only; b) Standard deviation of the error - IR data only; c) Mean error - combined IR and CIMR data; d) Standard deviation of the error - combined IR and CIMR data.

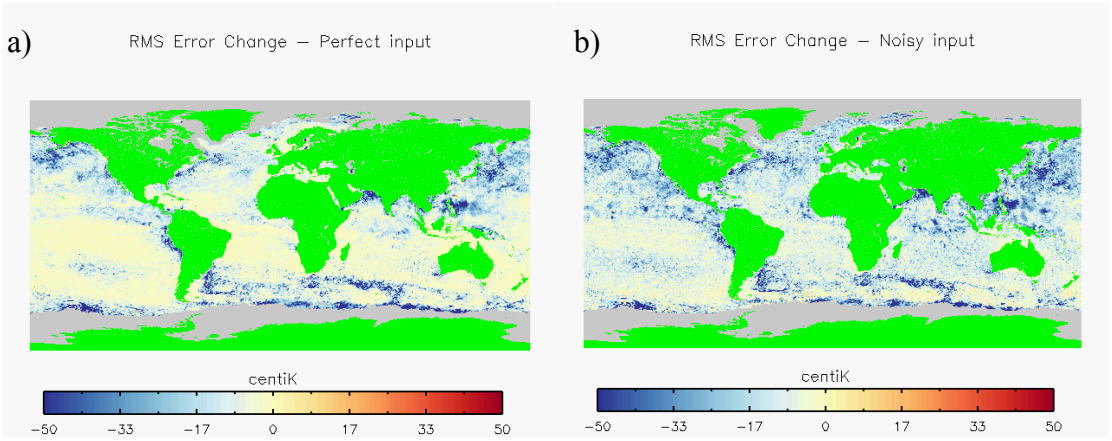

Figure 10 Change in the RMS error of the reconstructed SST field in July from adding CIMR data to the input for: (**a**) perfect input data; (**b**) input data containing realistic errors.

A summary of the RMSE in different regions for each of the configurations is given in Table 2. In validation of current operational OSTIA products, RMSE typically ranges 0.3-0.5[14], so the similar

magnitude of results in this table suggest that this simulation study is performing realistically. The addition of CIMR data results in a marked decrease in RMSE in all regions except the coast. The coastal region (defined as cells less than 25 km from land) shows only small improvements with the addition of the CIMR data. This is consistent with the restriction of the PMW observations to be greater than this distance from land. The minimisation step in the NEMOVAR algorithm, however, is able to spread some information spatially accounting for the small improvement. For the case of data with realistic errors, the addition of CIMR data results in the global mean RMSE decreasing from 0.369 to 0.210 in January and from 0.338 to 0.225 in July. Improvements of this magnitude in RMSE suggest CIMR should support a step-change improvement in daily SST analyses.

Table 2 Root-mean-square error in different regions for the various experimental configurations

	Configuration	Global	Aghulas Current	Gulf Stream	Maritime	Southern Ocean	Coast
Jan	Perfect IR-only	0.310	0.532	1.286	0.394	0.369	0.641
	Perfect IR+CIMR	0.175	0.312	0.358	0.212	0.132	0.608
	Realistic IR-only	0.369	0.587	1.289	0.462	0.396	0.667
	Realistic IR+CIMR	0.210	0.337	0.386	0.233	0.169	0.622
July	Perfect IR-only	0.338	0.325	0.410	0.236	0.493	0.981
	Perfect IR+CIMR	0.225	0.159	0.258	0.159	0.078	0.969
	Realistic IR-only	0.395	0.384	0.506	0.335	0.496	0.995
	Realistic IR+CIMR	0.249	0.199	0.284	0.200	0.130	0.969

3.2. Reconstruction in Dynamical regions

Figure 11 shows spatial power spectra of the SST fields from the January analysis using the data with realistic errors for the region of the Aghulas current and Gulf Stream. These are plotted as a ratio to the "truth" power spectra in these regions and so perfect replication of the truth field in these plots would give a ratio of 1:1 across the whole spectrum. In both cases there is a marked improvement in

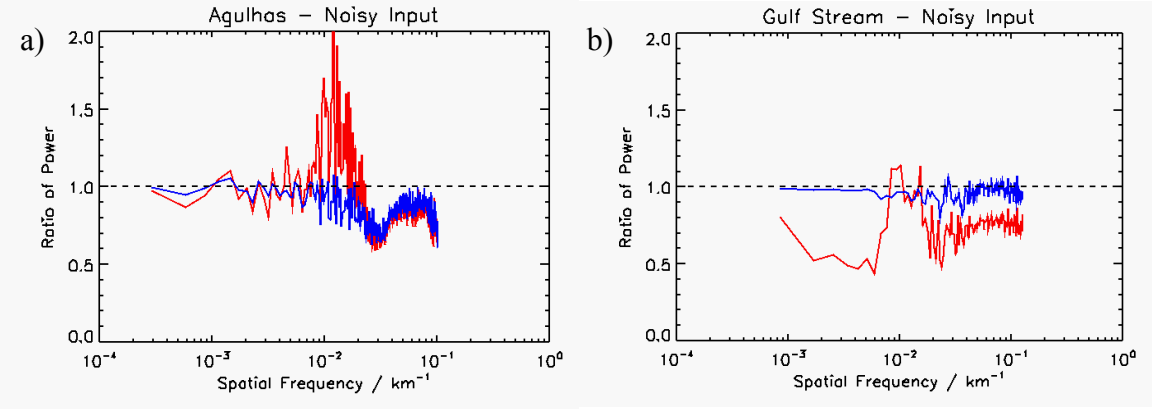

Figure 11 Comparison of the power spectra of the SST field in January from IR-only analysis (red) and combined IR and MW analysis (blue) where both contain realistic input errors. The data are plotted as a ratio to the "truth" SST power spectrum at each wavelength. (**a**) Aghulas Current region; (**b**) Gulf Stream region.

the agreement with the original "truth" dataset by the addition of CIMR data, as shown by the blue lines being closer to the 1:1 ratio across almost all spatial frequencies than the red lines.

The structure inherent in the SST fields in these regions is shown in Figure 12. This shows a map of the mean magnitude of the gradient of the SST field in the second-half of January. Figure 13 shows

the difference from these fields for the reconstructions using the input data with realistic errors. In many instances these difference maps show pairs of red and blue areas that would be expected from a spatial offset of a feature in the SST field. The area of these regions is much reduced by the addition of CIMR data. The fraction of cells where the magnitude of the difference is greater the 0.02 °C km^{-1} decreases from 6.6 % to 3.1% for the Aghulas Current and from 30.2% to 9.8% for the Gulf Stream. In some locations there are larger patches of difference eg. just left of centre in Figure 13 (a) and (c) and bottom left of Figure 13 (b) and (d). Here, in the IR-only case the interpolation scheme has produced structures not present in the "truth" dataset. These are artefacts resulting from interpolation of data that are too sparse. This limitation of optimal interpolation in regions with strong SST gradients was noted in the context of an AVHRR-only reconstruction by [30] and discussed more generally in [31]. With the sparser coverage of the IR-only case, the analysis only has input observations of these structures intermittently: the analysis gets to "see" the evolving structures on some days and reconstructs the features only at their locations on those days. The discrete nature of these locations persists in the time intervals without observations and ultimately becomes apparent in the mean over the period. The better coverage achieved with CIMR, improves the sampling so that there is a more representative set of positions for the structures over the period and thus a better representation of the mean field. These artefactual structures have been greatly reduced with the addition of CIMR data because the true structures are sampled at a resolution that usefully resolves their locations on most days.

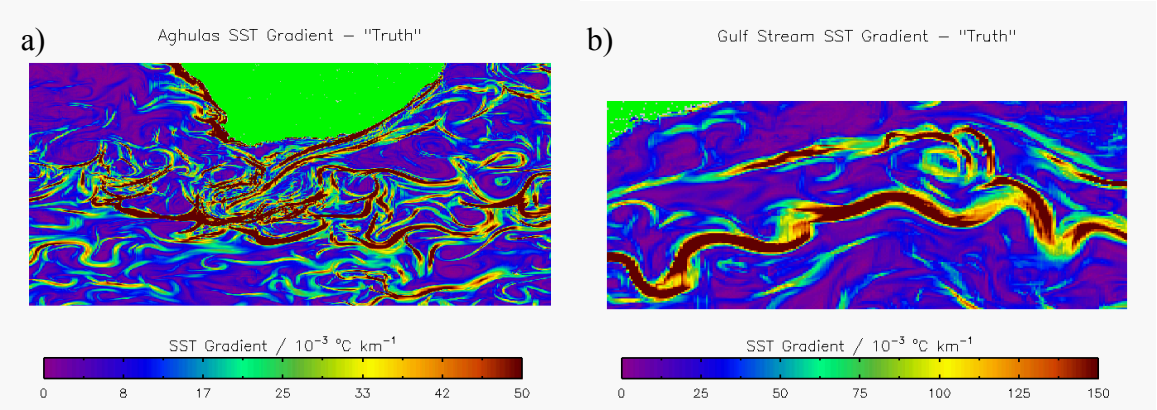

Figure 12 Gradient of the SST field in January in the "truth" data set for: (**a**) Aghulas Current region; (**b**) Gulf Stream region.

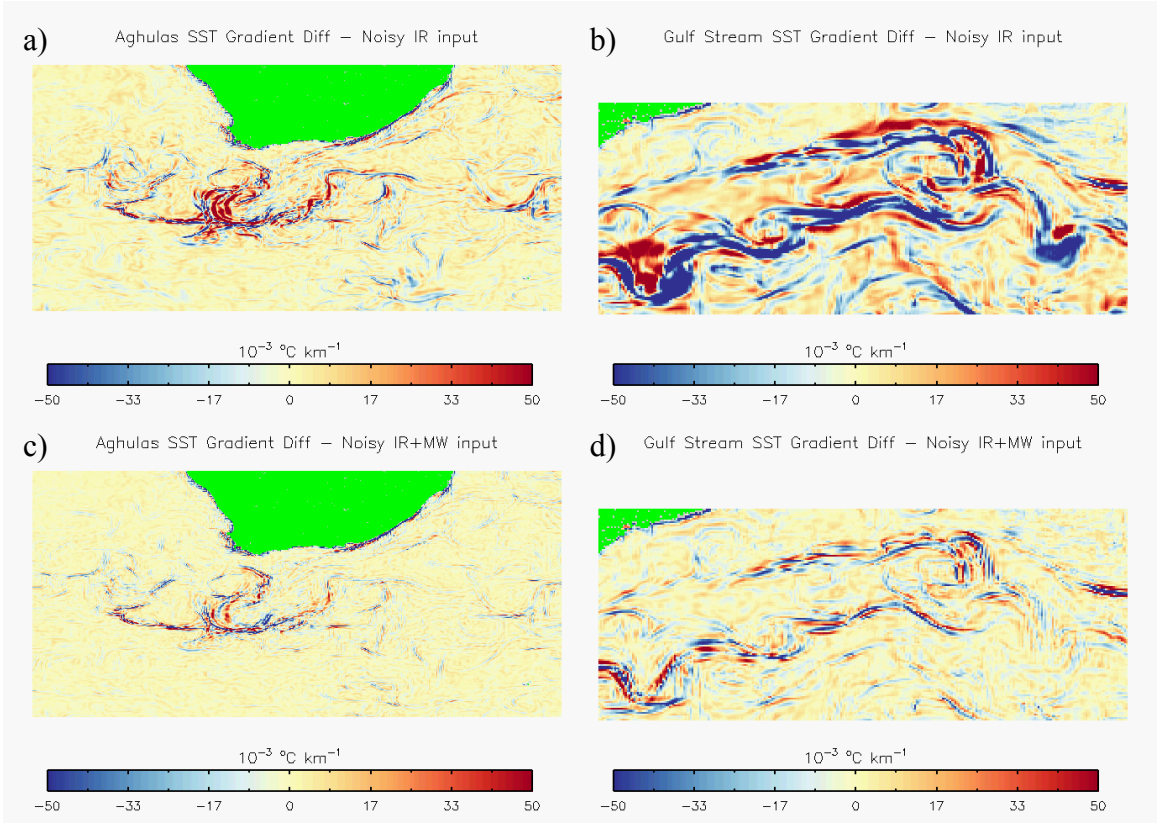

Figure 13 Difference from the "truth" SST gradient field in January for output of OSTIA reconstructions using input data with realistic errors: (**a**) IR-only data – Aghulas current region; (**b**) IR-only data- gulf stream region; (**c**) Combined IR and MW data – Aghulas current region; (**d**) Combined IR and MW data – Gulf stream region.

In summary, adding CIMR data to the IR constellation reduces both the mean error and error standard deviation globally. There is also clear improvement in areas of particular challenge such as around strong ocean temperature gradients and dynamics and regions of persistent cloud. The "perfect" data results show that this is a result of the improved coverage available from CIMR despite the lower weight given to each of the individual observations compared to the IR. The fact that this improvement remains when data with realistic errors is used show that this improvement will hold true when CIMR is added to an IR-only constellation in the future.

4. Conclusions

We have conducted an investigation into the effect of adding CIMR to an IR-only observing system on global analyses of SST. Adding CIMR resulted in a reduction in the global RMSE of SST in analysis data from 0.37 K to 0.21 K for January and 0.34 K to 0.23 K for July. There were also strong improvements in dyamical regions such as the Aghulas current (from 0.59 K to 0.39 K in January and 0.38 K to 0.20 K in July) and Gulf Stream (from 1.29 K to 0.39 K in January and 0.51 K to 0.29 K in July). There were noticeable examples of artefacts in the reconstruction being removed with the additional coverage provided by CIMR.

CIMR would make an important contribution to global observations of SST and result in a large reduction in the errors in analyses. Its near-daily coverage and ability to provide SST in the presence of clouds would significantly improve the analysis reconstruction of dynamical regions where there are strong SST contrasts and in regions with persistent cloud coverage.

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