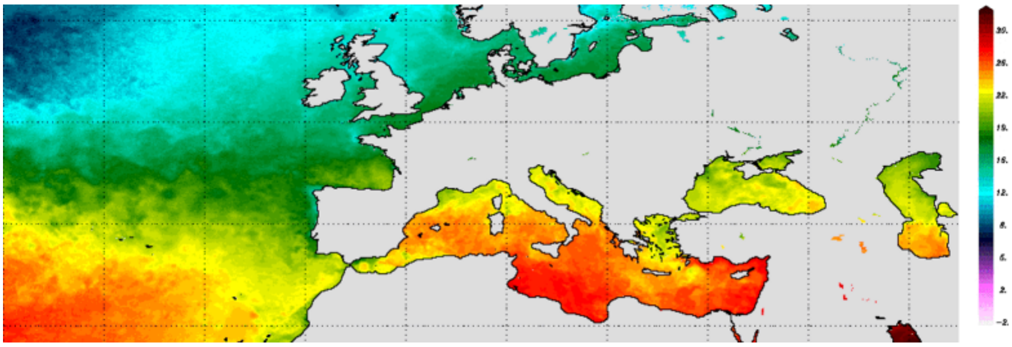
ESA CCI+ Phase 1 Sea Surface Temperature (SST)



Uncertainty Characterisation (E3UB) D2.2 v2

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List of Acronyms

AVHRR	Advanced Very High Resolution Radiometer
CCI	Climate Change Initiative
CDR	Climate Data Record
E3UB	End-to-end Error and Uncertainty Budget
ESA	European Space Agency
NWP	Numerical Weather Prediction
OE	Optimal Estimation
RTTOV	Radiative Transfer for TOVS
SST	Sea Surface Temperature
TBC	To be confirmed

1. SCOPE

This is a report in preparation for a comprehensive report on Uncertainty Budget (formally, End-to-End Error Evaluation and Uncertainty Budget, E3UB) that will be completed to describe the Sea Surface Temperature Climate Change Initiative Version 3 Climate Data Record (SST CCI v3 CDR). The full E3UB will be document E3UB D2.2 v3.

The form of content of this interim E3UB report is:

- presentation of error covariance estimates for use in SST retrieval and uncertainty evaluation

This development arose as part of algorithm development of bias-aware optimal estimation for AVHRR sensors. This algorithm development is described in the SST CCI Algorithm Theoretical Basis Document (ATBD) D2.1 v2.

2. UNCERTAINTY MODEL FOR OPTIMAL ESTIMATION

2.1 Introduction

Optimal estimation SST is used for AVHRR 2- and 3-channel retrievals in SST CCI in order to achieve known and satisfactory levels of SST sensitivity, by explicitly using prior NWP to address deficits in the window-channel information about the atmospheric influence on brightness temperatures. The OE solution is obtained in one step, because the retrieval context is adequately linear.

SST CCI (in phase 1) recognised that climate data record (CDR) uncertainties are complex in that contributing errors have a mix of spatio-temporal correlation length scales, and pioneered the principle of modelling uncertainty in three components:

(1) independent (also known as "random"), which is the component for which there is no correlation of errors between different SSTs; a typical source is the error from instrumental noise

(2) locally correlated, which is the component for which errors are strongly coupled for SSTs that are close in space and time, but become independent at large separations; a typical source is the error from ambiguity in retrieval under the specific atmospheric conditions observed

(3) large-scale correlated (including "systematic" or "common" errors), for which errors are coupled at large separations, including across the whole mission; a typical source is calibration error

Optimal estimation is a retrieval framework that provides an uncertainty estimate per retrieval. However, in previous SST CCI datasets, we have not been able simply to use these OE uncertainties, because their correctness relies on the OE being performed with realistic error covariance matrices, which, hitherto, have been poorly estimated. Somewhat ad hoc work-arounds have therefore been used.

However, as explained in Merchant et al. (2020a) and Merchant et al. (2020b) and ATBD D2.1 v2, we now have a theoretical basis on which to estimate proper error covariance matrices for OE. This basis is “bias-aware optimal estimation” As well as putting Bayesian cloud detection and SST retrieval on a firmer footing, this improve the OE uncertainty framework in the CDR v3 for SSTs in particular from Advanced Very High Resolution Radiometers (AVHRRs).

The classic OE formulation doesn't consider error correlation length scales or how to partition uncertainty into the three components. This has been addressed in E3UB D2.2 v1.

2.2 OE uncertainty

The uncertainty evaluation from an optimal estimation (OE) retrieval is:

$$\boldsymbol{S} = (\boldsymbol{K}^{\mathrm{T}}\boldsymbol{S}_{\epsilon}^{-1}\boldsymbol{K} + \boldsymbol{S}_{a}^{-1})^{-1} \qquad \text{Eq. 1}$$

The point of note here is that the retrieval uncertainty includes the observation-simulation error covariance matrix, $\boldsymbol{S}_{\epsilon}$, and prior error covariance (for the reduced state vector used for retrieval), $\boldsymbol{S}_{\boldsymbol{a}}$. If these matrices are poorly estimated, the uncertainty estimate will be biased. These error covariances are now more objectively estimated used BAOE and results are presented here for three AVHRR sensors, NOAA 8, 9 and 11.

2.3 Prior error covariance

The BAOE process is formulated such that independence of errors in prior SST and prior TCWV is assumed. The prior error covariance is therefore characterised by just two parameters, the SST and TCWV uncertainty. The estimates obtained via BAOE for these are shown in Table 1.

Table 1. Prior state uncertainty estimates

Sensor	Prior SST uncertainty / K	Prior TCWV uncertainty / kg m^{-2}
NOAA 08	0.53	3.0
NOAA 09	0.50	3.7
NOAA 11	0.44	4.0

The prior SST is the dust-bias-adjusted (Merchant & Embury, 2020) SST analysis from the version 2 SST CCI climate data record (CDR v2). For the period spanned by the BAOE analysis of these missions (1985 – 1990), the prior SST estimates are reasonable, and it is plausible that the uncertainty for the earlier sensor periods increases relative to the later mission.

For prior TCWV uncertainty the background knowledge regarding what to expect is much less, although estimates have been attempted by less objective techniques before

(Merchant, Le Borgne, Marsouin, & Roquet, 2008). The mean uncertainty estimate across the sensors, 3.6 kg m^{-2}, corresponds to 16% on average. Since there is a firm lower limit (TCWV is never negative) the treatment of this uncertainty within the processing chain is as a fractional uncertainty.

The prior TCWV uncertainty is not known or expected to have any temporal tendency for this period. It should not depend on sensor, and the spread is interpreted as uncertainty in the uncertainty estimate. This may become clearer as more sensors in the series are analysed.

2.4 Observation-simulation error covariance

The BAOE is performed on BTs averaged over between 5 and 25 clear-sky pixels, which reduces the instrument noise. The evaluation of $\boldsymbol{S}_\epsilon$ is therefore assumed to be dominated by fluctuations (to some degree in common between channels) in calibration and in the simulation, rather than noise. For evaluating the per-pixel uncertainty in the SST CCI processor, the internally generated noise (NEDT) estimates for each channels is added to the error covariance matrices described here: this has the effect of adding to the diagonal terms of the matrix only, since noise is independent between channels.

The uncertainty in the observations (to which noise will be added for pixel resolution work) has been evaluated within the BAOE framework as a function of slant-column water vapour path (WVP). This reflects the hypothesis that the most likely source of error to have a systematic dependency is in the simulation: as the atmosphere becomes less IR-transparent, but uncertainty is likely to increase in window channels – whether because of more column mass of water vapour or because a given mass is view at an oblique angle.

The uncertainty associated with NOAA 08 is, as expected, rather higher than the two later sensors. For NOAA 09 and 11, only the 12 um channels have a clear dependence on WVP, increasing for atmospheres with greater paths, as expected. The results for NOAA 09 and 11 are consistent with each other, which may reflect that these are the same AVHRR instrument version, in distinction to NOAA 08.

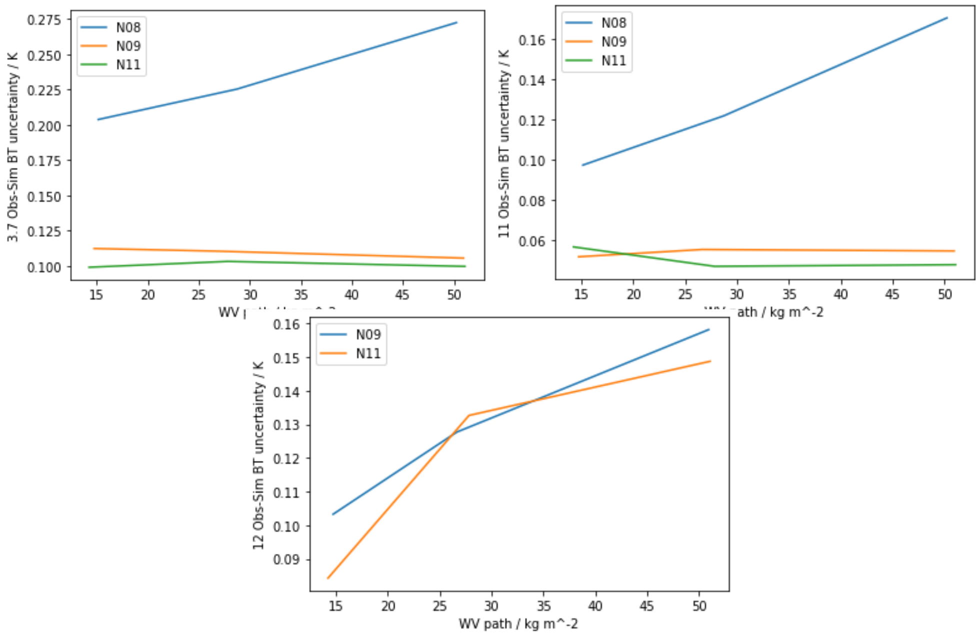

Figure 1. Uncertainty estimates for observations parameterised against WVP.

For appropriate evaluation of uncertainty, error correlations are also important. These correlations may arise from common effects in calibration or simulation. The error correlations obtained for NOAA 8 between its two channels is high, being 0.89.

The results for NOAA 09 and NOAA 11 are shown in Table 2, and are highly consistent between the two. Whether this reflects commonality in the instruments or their radiative transfer simulations is a question to be understood.

Table 2. Error correlations between channels.

Correlation between	NOAA 09	NOAA 11
3.7 - 11	0.13	0.17
11 - 12	0.21	0.24
12 - 37	0.36	0.34

3. CONCLUSIONS

First BAOE results on error covariances suggest significant differences between the error characteristics of NOAA 08 and two later AVHRRs, which will be reflected in the associated uncertainty estimates of derived SSTs. Results are plausible for and consistent between NOAA 09 and NOAA 11. Interchannel error correlations are generally low, which is a positive insight for SST retrieval (since channel differences are key to the retrieval outcome).

4. REFERENCES

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