Single Sensor Error Statistics

Report for (A)ATSR L2P Project:
WP 11 – D 1.1
WP 41 – D 4.1

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Accepted by: N. Houghton ……..

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Document Control

Version Number:	Comment:	Issued to:
1A	Draft for comment and for WP 53	M. Pritchard B. Maddison H. Kelliher C. Donlon
1B	Updated draft for comment and for WP 53 following feedback from C. Donlon.	M. Pritchard B. Maddison H. Kelliher C. Donlon
1C	Updated following feedback from H. Kelliher.	M. Pritchard B. Maddison H. Kelliher C. Donlon N. Houghton
1D	Updated draft with SSES analysis	H. Kelliher
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1F	Updated with SSES for ATSR-1 Updated with robust statistics	H. Kelliher
2A	Updated following feedback from H. Kelliher. New issue for Final Review.	M. Pritchard B. Maddison H. Kelliher N. Houghton

1 EXECUTIVE SUMMARY

This document contains the specification for Single Sensor Error Statistics (SSES) for the L2P project. The document summaries the inputs, methodology for producing SSES and output L2P file format definitions, for ATSR-1, ATSR-2 and AATSR.

1.1 Inputs

The required inputs for the document are:

Documentation:

AD1: An updated Confidence Flagging Scheme for Medspiration AATSR L2P Files, MED-UL-REP-001, Issue 2B, 18/11/2007.

AD2: An updated Confidence Flagging Scheme for Medspiration AATSR L2P Files, MED-UL-REP-002, Issue 1D, 17/03/2008.

AD3: The Recommended GHRSTT-PP Data Processing Specification (GDS), Version 1 Revision 1.7, 09/05/2007.

AD4: Document defining format of the database of (A)ATSR matchups, D 3.3.

AD5: Donlon, C.J., P.J. Minnett, C. Gentemann, et al., 2002. Toward Improved Validation of Satellite Sea Surface Skin temperature Measurements for Climate Research, J. Climate, 15, 353-369.

AD6: Merchant C. J., Horrocks L. A., Eyre J., and O'Carroll A. G., 2006. Retrievals of sea surface temperature from infra-red imagery: origin and form of systematic errors, Quart. J. Royal Met. Soc., 132, 1205-1223.

AD7: Merchant C. J., and Harris A.R., 1999. Toward the elimination of bias in satellite retrievals of skin sea surface temperature. 2: Comparison with in situ measurements, J Geophys Res, 104, C10, 23579-23590.

AD8: Analytical Methods Committee, 2001. Robust Statistics: a method of coping with outliers. AMC Technical Briefs - ISSN 1757-5958, No 6.

Data sets:

DS1: The Medspiration match-up database (MDB) for AATSR.

DS2: The L2P MDB for (A)ATSR, D 3.2.

DS3: The Database of global SSES fields for all ATSR-1, ATSR-2 and AATSR data mapped to all SST retrievals from 1991 – June 2003, D4.1.

1.2 Outputs

The output is the specification and derivation of SSES for ATSR-1, ATSR-2 and AATSR.

2 INTRODUCTION

The SSES scheme developed for AATSR by UL for Medspiration forms the basis of the SSES updated scheme to be used in this project [AD1, AD2]. The SSES scheme requires a match-up database of satellite versus in situ buoy data as defined by GHRSST-PP [AD3].

The L2P project will:

- Seek to improve on the current AATSR SSES by using an in situ data set with higher Quality Control (QC)
- Seek to improve on the current AATSR SSES by accounting for temporal and spatial variations of the SSES
- Provide the first set of SSES for ATSR-1 and ATSR-2

2.1 Scope of this document

The L2P project will convert the entire (A)ATSR data set from 1991 to date to GHRSST-PP L2P format and will therefore need a MDB covering this period. This document describes the methodology for producing, and derivation of, the SSES for ATSR-1, ATSR-2 and AATSR. It describes how the SSES should be included in the L2P files. The document assumes complete familiarity with (A)ATSR data in both L2P and Envisat formats.

3 SINGLE SENSOR ERROR STATISTICS

The aim of the Global Ocean Data Assimilation Experiment (GODAE) High Resolution Sea Surface Temperature Pilot Project (GHRSST-PP) is to develop and operate an internationally distributed system that delivers a new generation of high-resolution (better than 10 km) global coverage SST data products in a near real-time (NRT, ~6 hourly) operational context during 2005-2008. The GHRSST-PP L2P data files contain SST level 2 data as generated by the agency responsible for its original production. To these are added additional ancillary data such as wind speed, solar insolation and aerosol optical depth, as specified in AD3. These ancillary data are intended to help the user filter and interpret the SST data. In other words, the ancillary data should provide information that enables users to develop and carry out their own quality control procedures appropriate to their particular application.

In addition, it is necessary to provide uncertainty estimates for all retrievals in the form of sensor specific error statistics (referred to as GHRSST-PP SSES values). A bias and standard deviation is assigned to each pixel individually, along with a confidence flag (a value between 0 and 5) referred to as the Proximity Confidence Value (PCV). The rationale for assigning errors individually to every pixel is to allow a distinction to be made between pixels that are more or less likely to be at risk of error. For different sensors different factors contribute to that risk. The task of assigning SSES to each pixel consists of assessing the likelihood of error according to the risk factors determined for a particular SST product. The susceptibility to error is stratified into several PCVs as summarised in Table 3.1. Each of levels for good data (levels 2 to 5) is associated with a range of standard deviations derived from analyses of validation datasets in which satellite data are matched to coincident in situ measurements.

Table 3-1: Confidence values for L2P SST values and their intended meaning

Proximity Confidence Value	What it Represents
0	No data (unprocessed, land etc.)
1	No SST data (cloud etc.)
2	Bad data
3	Marginal quality
4	Good quality data
5	Excellent quality data

3.1 Current Methodology

The current SSES scheme for AATSR was developed as part of the Medspiration project. The derivation of the scheme is summarised in AD1 and the determination of the SSES is summarised in AD2. The scheme uses a 12-fold stratification of the MDB based on thresholds derived from an analysis of dual-view minus nadir-only SST differences according to the following table.

Table 3-2: Summary of D-N stratification.

If D2 Retrieval	If D3 Retrieval
TL_2 < D-N < TU_2	TL_3< D-N < TU_3
D-N < TL_2	D-N < TL_3
D-N > TU_2	D-N > TU_3

In addition, as AATSR provides estimate of the skin SST and the SSES are calculated from comparisons to a depth SST measured by surface drifting buoys, each of the 6 classifications given above is further split by a single wind speed threshold of 6 ms^{-1} according to the recommendations given in AD5. This results in a 12-fold stratification scheme for analysis of the MDB, as shown in Table 3-3.

Table 3-3: Stratification Cases

Stratification Case	Summary of criteria		
Case 1:	2-channel	TL_2 < **D-N** < TU_2	Wind < 6ms^{-1}
Case 2:	2-channel	TL_2 < **D-N** < TU_2	Wind > 6ms^{-1}
Case 3:	2-channel	**D-N** < TL_2	Wind < 6ms^{-1}
Case 4:	2-channel	**D-N** < TL_2	Wind > 6ms^{-1}
Case 5:	2-channel	**D-N** > TU_2	Wind < 6ms^{-1}
Case 6:	2-channel	**D-N** > TU_2	Wind > 6ms^{-1}
Case 7:	3-channel	TL_3 < **D-N** < TU_3	Wind < 6ms^{-1}
Case 8:	3-channel	TL_3 < **D-N** < TU_3	Wind > 6ms^{-1}
Case 9:	3-channel	**D-N** < TL_3	Wind < 6ms^{-1}
Case 10:	3-channel	**D-N** < TL_3	Wind > 6ms^{-1}
Case 11:	3-channel	**D-N** > TU_3	Wind < 6ms^{-1}
Case 12:	3-channel	**D-N** > TU_3	Wind > 6ms^{-1}

3.2 Potential Improvements to Current Methodology

The current SSES scheme uses global statistics calculated using all match-ups collated into the MDB. It is likely that regional and/or temporal variations exist within these global statistics, and so several analyses of the MDB were carried out to see if the SSES for AATSR could be improved to account for regional and temporal variations.

In the following analysis, only match-up cases that fall within the 3-sigma D-N thresholds are considered, i.e. Case 1, Case 2, Case 7 and Case 8. The number of match-ups for all other cases is not considered to be sufficient for further stratification.

3.2.1 Temporal Dependency of Matchup Database

The temporal variation of match-ups in the Medspiration MDB is evaluated by looking at how the observed difference between AATSR and drifting buoys varies over time. The temporal distribution of match-ups for Case 1, Case 2, Case 7 and Case 8 is shown below.

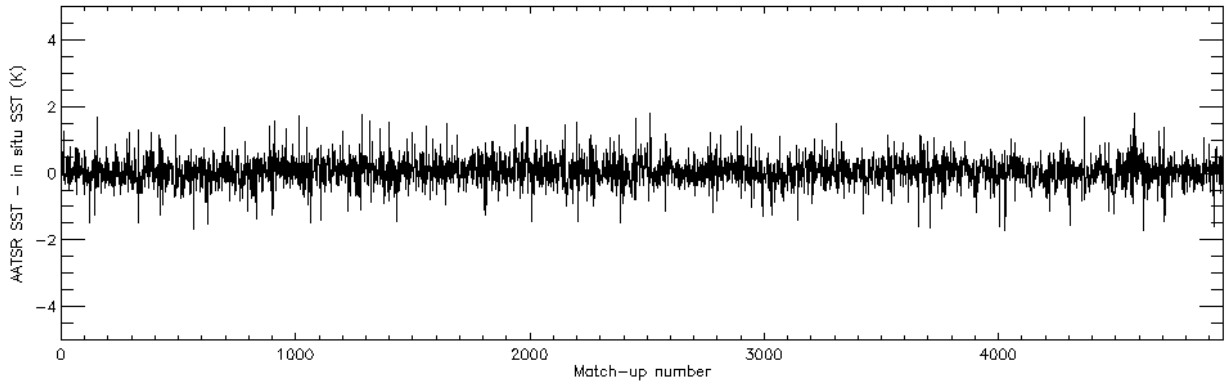

Figure 3-1: Temporal variation of Case 1 match-ups.

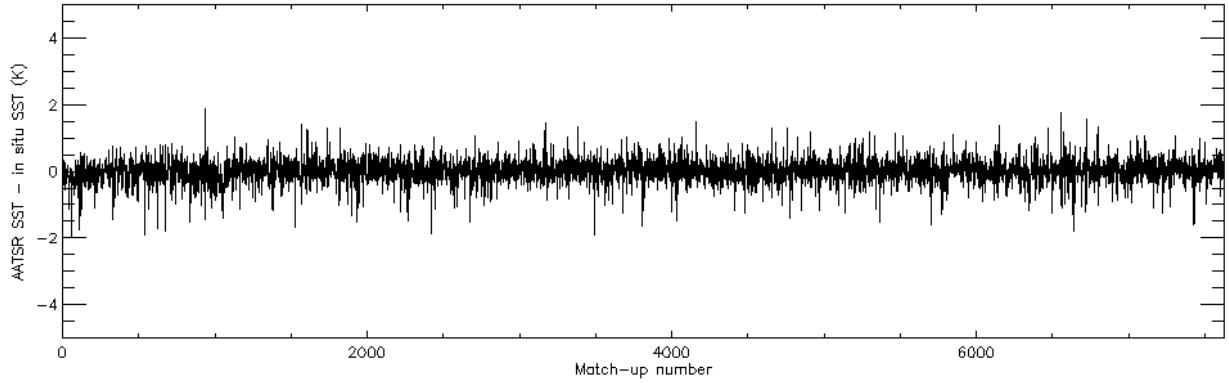

Figure 3-2: Temporal variation of Case 2 match-ups.

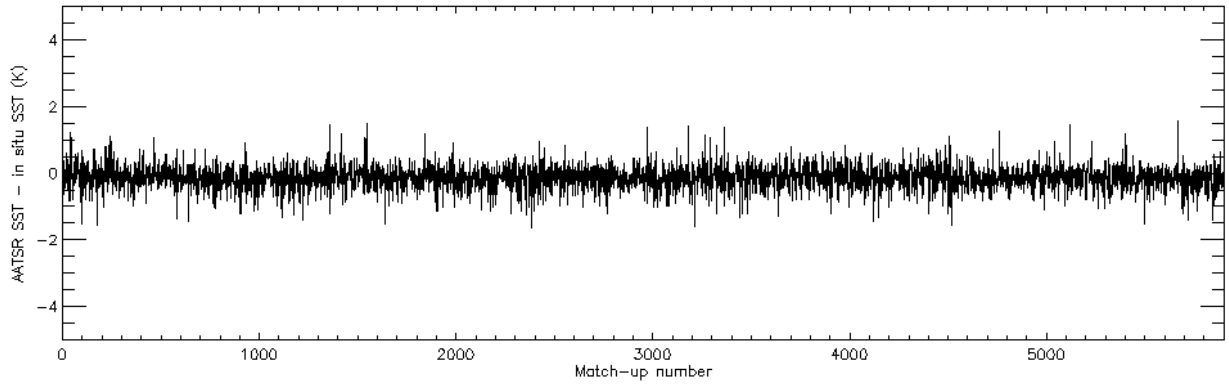

Figure 3-3: Temporal variation of Case 7 match-ups.

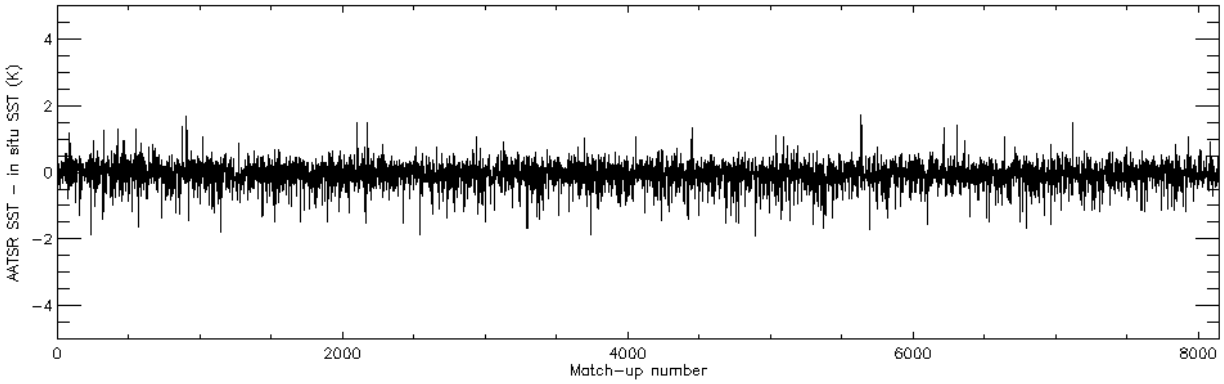

Figure 3-4: Temporal variation of Case 8 match-ups.

The temporal variation in figures 3-1 to 3-4 is shown as a function of match-up number, which is a proxy for time as the match-ups are stored chronologically in the MDB. As can be seen in all cases, the long-term stability of the match-ups is excellent, with no noticeable drifts or features in the time series. Consequently, we do not expect the global biases to vary significantly with time, and so no additional temporal dependency will be included in the SSES scheme.

3.2.2 Latitudinal Dependency of Matchup Database

The next dependency to be evaluated is the latitudinal dependency, as the (A)ATSR D2 SST retrievals are known to have a latitude dependent bias compared to the D3 SSTs [AD6]. The latitudinal dependency has been assessed by calculating the mean difference of all match-ups within 5-degree latitude bands from the South Pole to the North Pole. The results are given below for Case 1, Case 2, Case 7 and Case 8 match-ups.

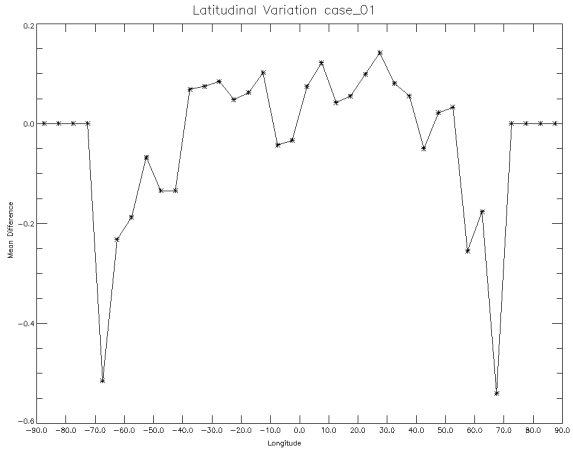

Figure 3-5: Mean bias for Case 1 match-ups averaged into 5-degree latitude bands.

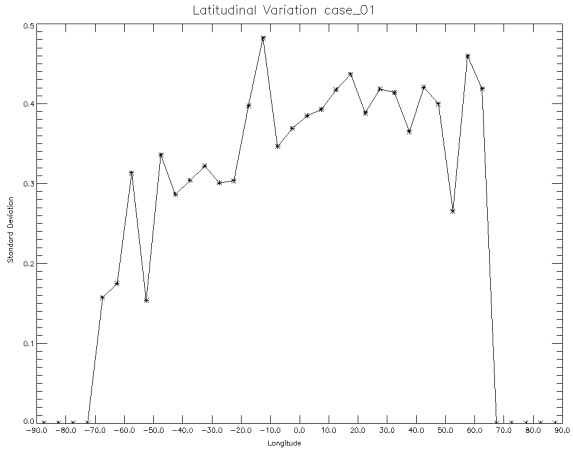

Figure 3-6: Standard deviation for Case 1 match-ups averaged into 5-degree latitude bands.

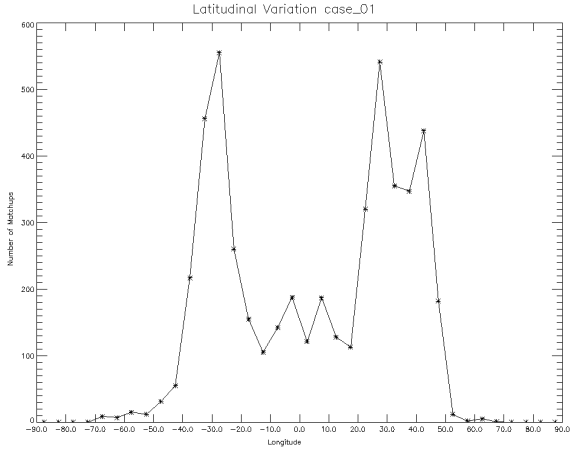

Figure 3-7: Number of match-ups for Case 1 match-ups averaged into 5-degree latitude bands.

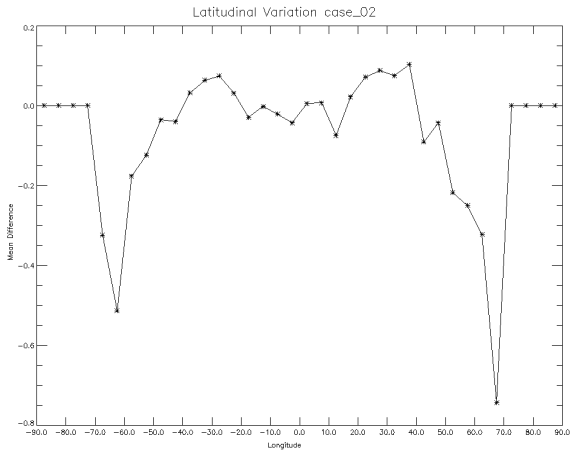

Figure 3-8: Mean bias for Case 2 match-ups averaged into 5-degree latitude bands.

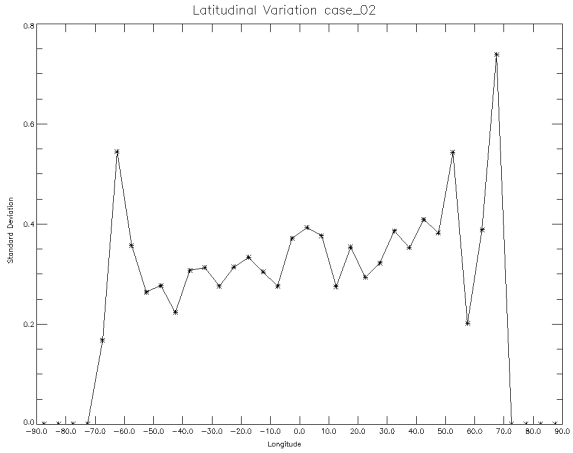

Figure 3-9: Standard deviation for Case 2 match-ups averaged into 5-degree latitude bands.

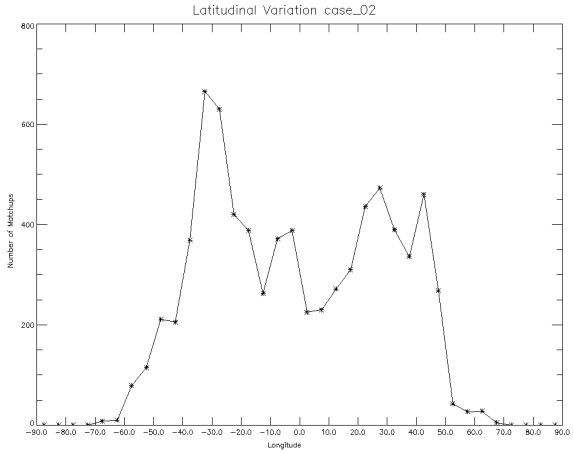

Figure 3-10: Number of match-ups for Case 2 match-ups averaged into 5-degree latitude bands.

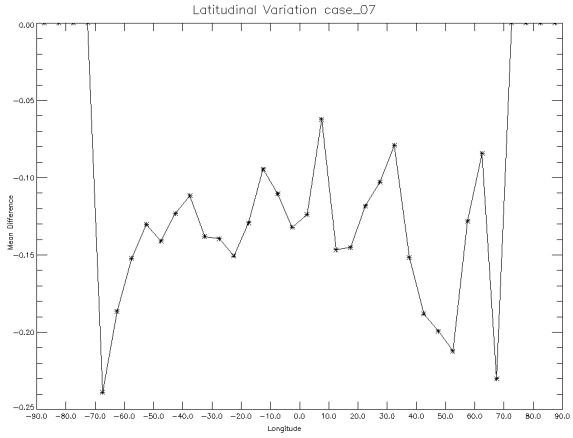

Figure 3-11: Mean bias for Case 7 match-ups averaged into 5-degree latitude bands.

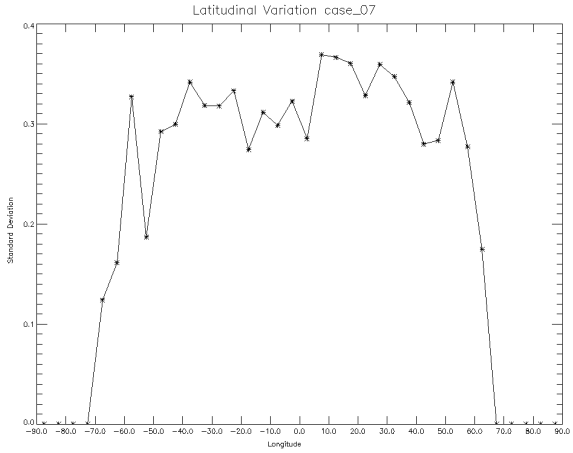

Figure 3-12: Standard deviation for Case 7 match-ups averaged into 5-degree latitude bands.

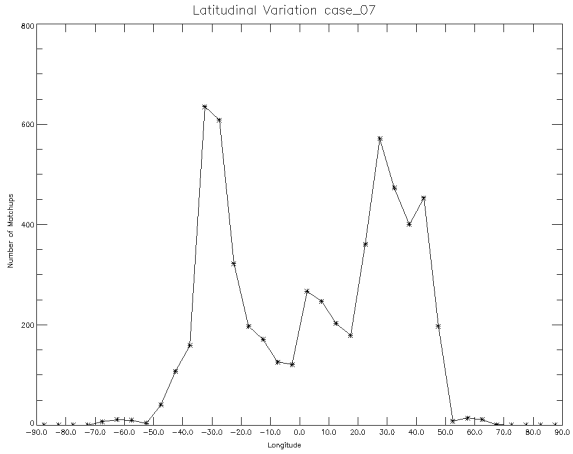

Figure 3-13: Number of match-ups for Case 7 match-ups averaged into 5-degree latitude bands.

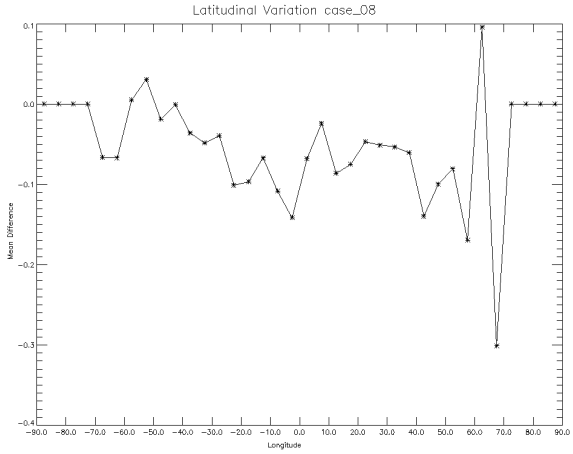

Figure 3-14: Mean bias for Case 8 match-ups averaged into 5-degree latitude bands.

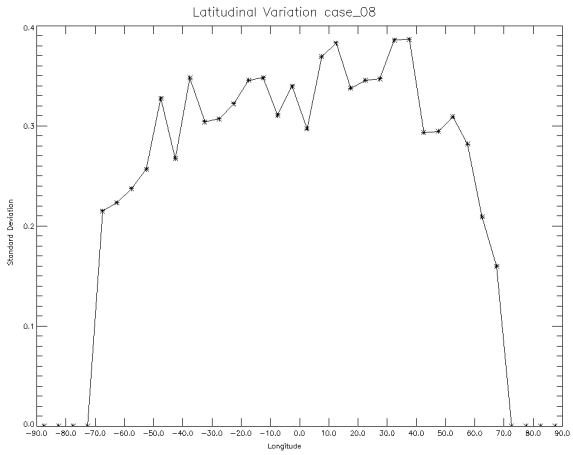

Figure 3-15: Standard deviation for Case 8 match-ups averaged into 5-degree latitude bands.

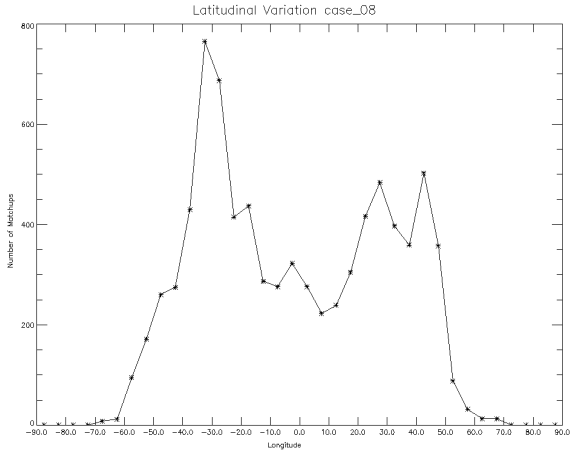

Figure 3-16: Number of match-ups for Case 8 match-ups averaged into 5-degree latitude bands.

Analysis of figures 3-5 to 3-16 indicates that:

- A latitudinal variation exists for both 2-channel and 3-channel retrievals.
- The 2-channel retrievals show a symmetrical bias centred on the Equator, with a strong decrease in the bias towards both poles. However, analysis of the number of match-ups suggests that the calculated high latitude biases might not be statistically significant. The magnitude of the bias is ~ 0.3 K between 60 ºN and 60 ºS.
- The 2-channel retrievals appear to show the "albatross-like" signature of the D2-D3 latitudinal bias reported in AD6.
- The 3-channel retrieval has a decrease in the bias above 50 º in both hemispheres, and has an approximate linear decrease from 50 ºS to 50 ºN; it is noted that the Case 7 plot is very noisy but an underlying linear decrease is apparent. The magnitude of the bias is around 0.1 K between 60 ºN and 60 ºS.
- The 3-channel retrievals show a clear offset in the bias between low wind speed and high wind speed match-ups.
- The distribution of match-ups for both 2-channel and 3-channel retrievals shows most match-ups occur between 20 º and 40 º in both hemispheres, with a more even distribution of match-ups between hemispheres observed during the day than at night.

The observation of the D2-D3 bias in the 2-channel retrievals is not surprising, and so a further correction could be made to include the D2-D3 offset if required. The linear dependency of the D3 retrievals is not understood and requires further analysis.

3.2.3 Basin Dependency of Matchup Database

The OSTIA analysis system uses a set of major oceanic basins for error analysis. These are:

- North Atlantic
- North Pacific
- South Pacific
- South Atlantic
- Mediterranean Seas
- Arctic Ocean
- Southern Ocean
- Indian Ocean
- Other significant seas

The basins are shown schematically in the next figure.

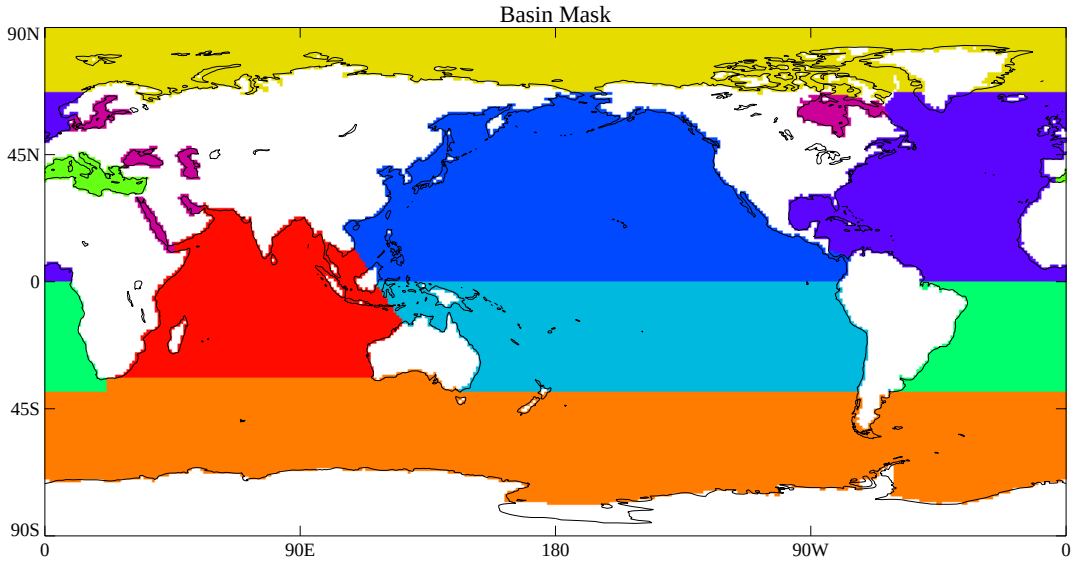

Figure 3-17: Location of major oceanic basins used for error analysis by OSTIA. (Image provided by John Stark, Met Office).

The mean bias, standard deviation and number of match-ups for each match-up case, for individual basins are shown below in Table 3-4.

Table 3-4: Statistical analysis of MDB, for major oceanic basins, for match-up cases 1, 2 7 & 8.

Basin	Case 1			Case 2			Case 7			Case 8		
	Bias	Sigma	Num	Bias	Sigma	Num	Bias	Sigma	Num	Bias	Sigma	Num
NA	+0.047	0.40	1586	+0.008	0.38	1996	-0.142	0.32	2071	-0.080	0.35	2345
NP	+0.105	0.41	756	+0.210	0.34	1228	-0.086	0.34	844	-0.050	0.33	1030
SP	+0.073	0.36	929	+0.168	0.33	1681	-0.136	0.30	771	-0.092	0.35	1231
SA	+0.030	0.31	844	+0.038	0.28	1194	-0.139	0.32	1144	-0.065	0.31	1526
MS	+0.061	0.39	277	+0.012	0.38	191	-0.197	0.30	248	-0.144	0.27	206
AO	-0.540	-	1	-	-	0	-0.230	-	1	-0.276	0.16	9
SO	-0.095	0.31	192	-0.077	0.29	799	-0.124	0.30	268	-0.010	0.29	1059
IO	+0.076	0.38	357	+0.028	0.38	534	-0.093	0.35	539	-0.054	0.32	731
O	+0.146	0.30	17	+0.131	0.04	4	-0.301	0.26	17	-0.213	0.13	9

The results in Table 3-4 indicate:

- There is a significant variation in the number of match-ups in each basin
- There is good agreement in the calculated statistics for seven of the nine regions for D3 retrievals, namely the North Atlantic, North Pacific, South Pacific, South Atlantic, Mediterranean Sea, Southern Ocean and Indian Ocean regions.
- There is good agreement in the calculated statistics for six of the nine regions for D2 retrievals, with the Southern Ocean results showing day time biases that are more consistent with the night time biases for the same region.
- The Arctic Ocean basin results indicate a cool bias for both D2 and D3 retrievals, although the number of match-ups is very small. However, the D3 bias is in reasonable agreement with the other basins.
- The seas classed as “other” show a strong positive bias for D2 retrievals and a strong negative bias for D3 retrievals, although the number of match-ups is very small.

The current inter-basin consistency suggests that no extra allowance for a basin dependency should be included in the SSES at this stage. However, further investigation of the D2 Arctic Ocean match-ups (when more become available) and all match-ups for the seas classed as “other” is recommended.

3.3 AATSR SSES

As summarised in section 3.1, the SSES scheme for AATSR was developed for Medspiration, and involves a 12-fold stratification of the MDB, based on the D-N SST difference and wind speed. This section summarises the calculation of the D-N thresholds, analysis of the MDB and determination of the SSES.

3.3.1 Calculation of D-N thresholds

The D-N thresholds for AATSR were derived for updated Medspiration L2P AATSR SSES scheme, and are documented in AD1. The thresholds are:

- TU_2 = + 0.04 ± 0.09 K
- TL_2 = - 1.53 ± 0.09 K
- TU_3 = + 0.51 ± 0.07 K
- TL_3 = - 0.51 ± 0.07 K

3.3.2 Analysis of MDB

A MDB of coincidences between AATSR and buoys was created using the methodology described in AD4. Owing to the delay in reprocessing AATSR to version 2.0, only a limited set of data was available for analysis. This data covered the periods December 2005 to February 2006, August 2006 to February 2007 and August 2007 to December 2007, 15 months in total. In the following case-by-case analyses of match-up data stratified into the 12 categories defined in section 3.1, a ± 3 sigma filter is applied before calculating the mean bias and standard deviation. This removes any remaining outliers that would otherwise overly affect the statistics. The ± 3 sigma limit means the statistics are representative of 99.87% of the match-up data.

In addition, the proposal of Merchant and Harris [AD7] to adopt robust statistics to alleviate the influence of outliers is implemented. An updated robust statistical scheme using Huber's method [AD8] is implemented, which provides a median and robust standard deviation for all analyses. If the range of variances follows Gaussian statistics then the resulting median and robust standard deviation will be very similar to the conventional mean and standard deviation.

Case 1: 2-channel retrieval; TL_2 < D-N < TU_2, wind speed < 6 m^{-1}

Figure 3-18 shows (a) the spatial distribution of Case 1 match-ups, (b) the histogram of the match-ups (together with a fitted Gaussian), and (c) a time series of the differences between AATSR and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

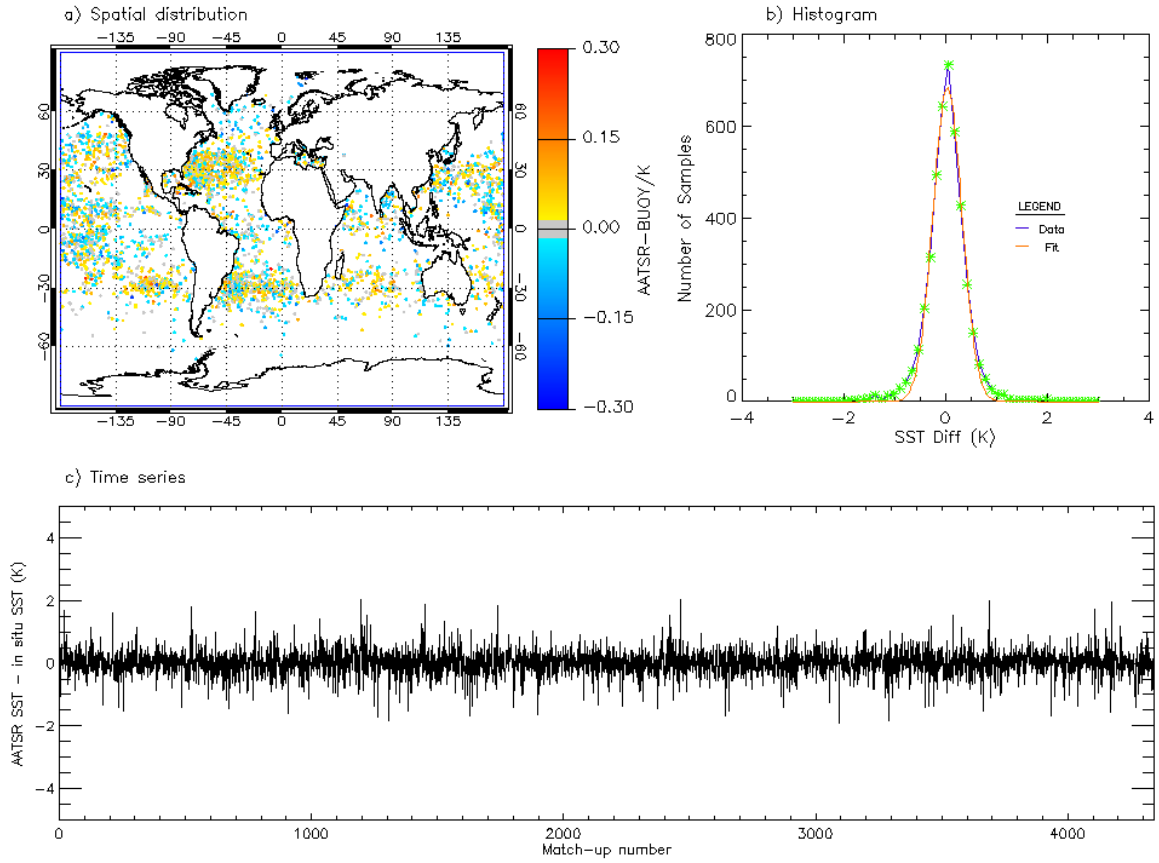

Figure 3-18: Spatial distribution, histogram and time series of Case 1 match-ups, 2-channel retrieval, TL_2 < D-N < TU_2, wind speed < 6 m^{-1}

The statistics for the Case 1 match-ups are given in Table 3-5. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-5: Statistics for Case 1 match-ups

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	4394	+0.022	0.38	+0.030	0.33
Moored only	708	-0.131	0.64	-0.129	0.54
Ships only	1742	-0.052	1.39	-0.141	1.17
TTP* only	184	+0.010	0.32	+0.010	0.31

*TTP = TAO/TRITON/PIRATA moored buoys

3.3.3 Case 2: 2-channel retrieval, $TL_2 < D\text{-}N < TU_2$, wind speed > 6 m^{-1}

Figure 3-19 shows a) the spatial distribution of Case 2 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between AATSR and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

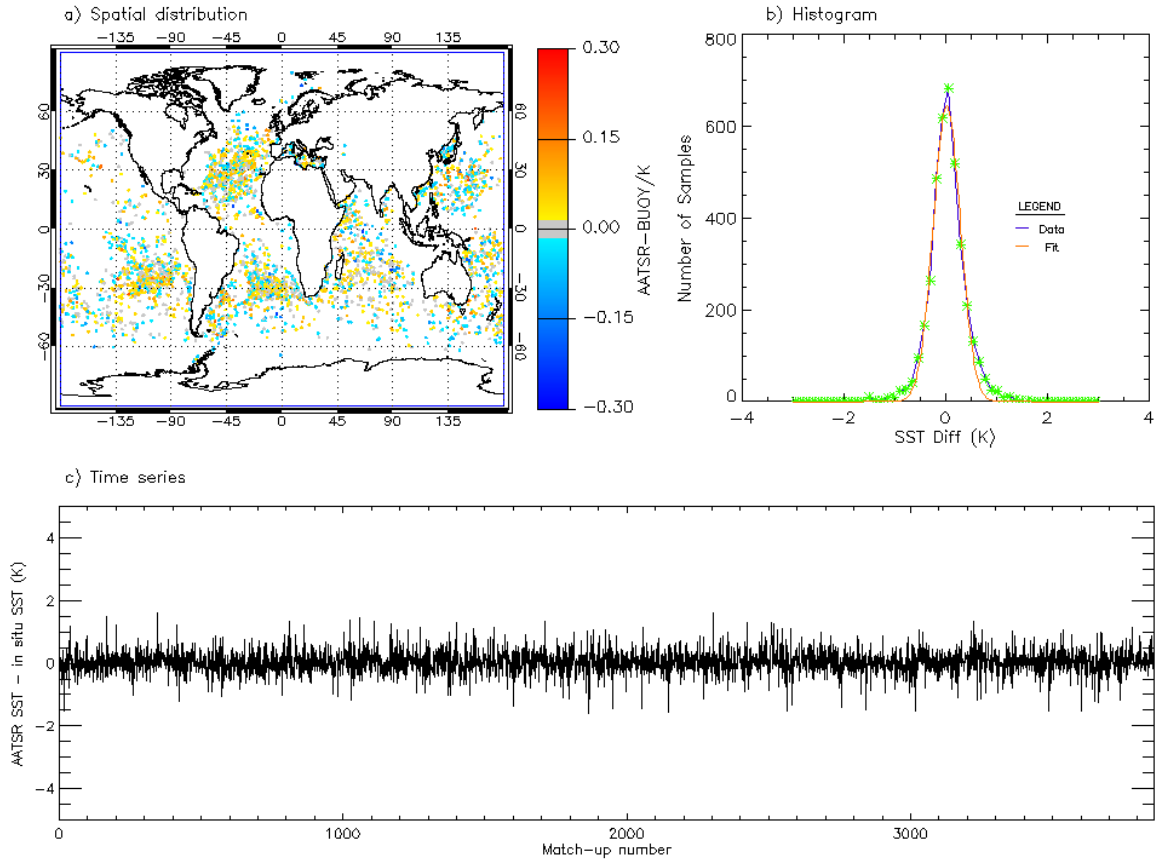

Figure 3-19: Spatial distribution, histogram and time series of Case 2 match-ups, 2-channel retrieval, $TL_2 < D\text{-}N < TU_2$, wind speed > 6 m^{-1}

The statistics for the Case 2 match-ups are given below. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-6: Statistics for Case 2 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	3907	+0.034	0.36	+0.022	0.32
Moored only	176	-0.201	2.11	+0.059	0.58
Ships only	1625	-0.167	1.38	-0.180	1.16
TTP* only	51	+0.033	0.30	+0.022	0.30

*TTP = TAO/TRITON/PIRATA moored buoys

3.3.4 Case 3: 2-channel retrieval, D-N < TL_2, wind speed < 6 m^{-1}

Figure 3-20 shows a) the spatial distribution of Case 3 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between AATSR and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

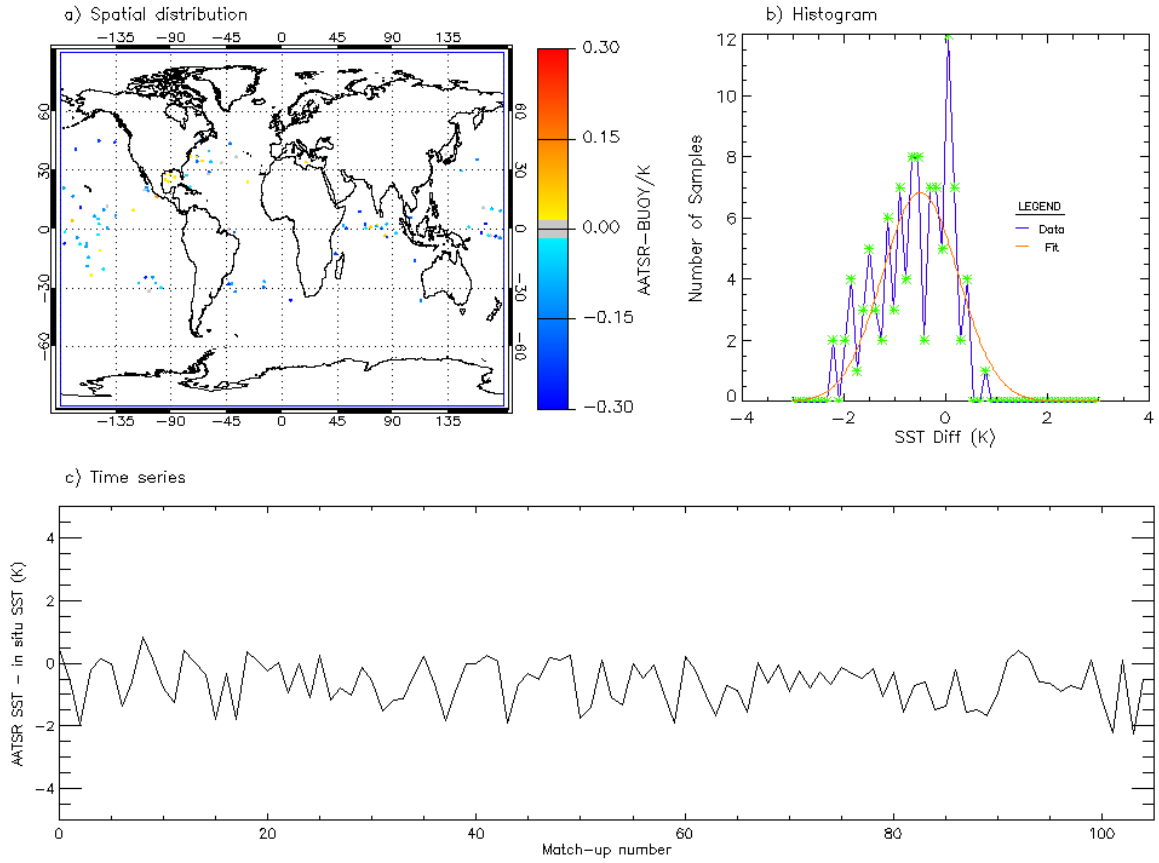

Figure 3-20: Spatial distribution, histogram and time series of Case 3 match-ups, 2-channel retrieval, D-N < TL_2, wind speed < 6 m^{-1}

The statistics for the Case 3 match-ups are given below. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-7: Statistics for Case 3 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	110	-0.625	0.70	-0.580	0.72
Moored only	27	-0.526	0.76	-0.430	0.79
Ships only	46	-0.952	1.49	-0.670	1.49
TTP* only	8	-0.669	0.83	-0.495	0.85

*TTP = TAO/TRITON/PIRATA moored buoys

3.3.5 Case 4: 2-channel retrieval, D-N < TL_2, wind speed > 6 m^{-1}

The figure below shows a) the spatial distribution of Case 4 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between AATSR and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

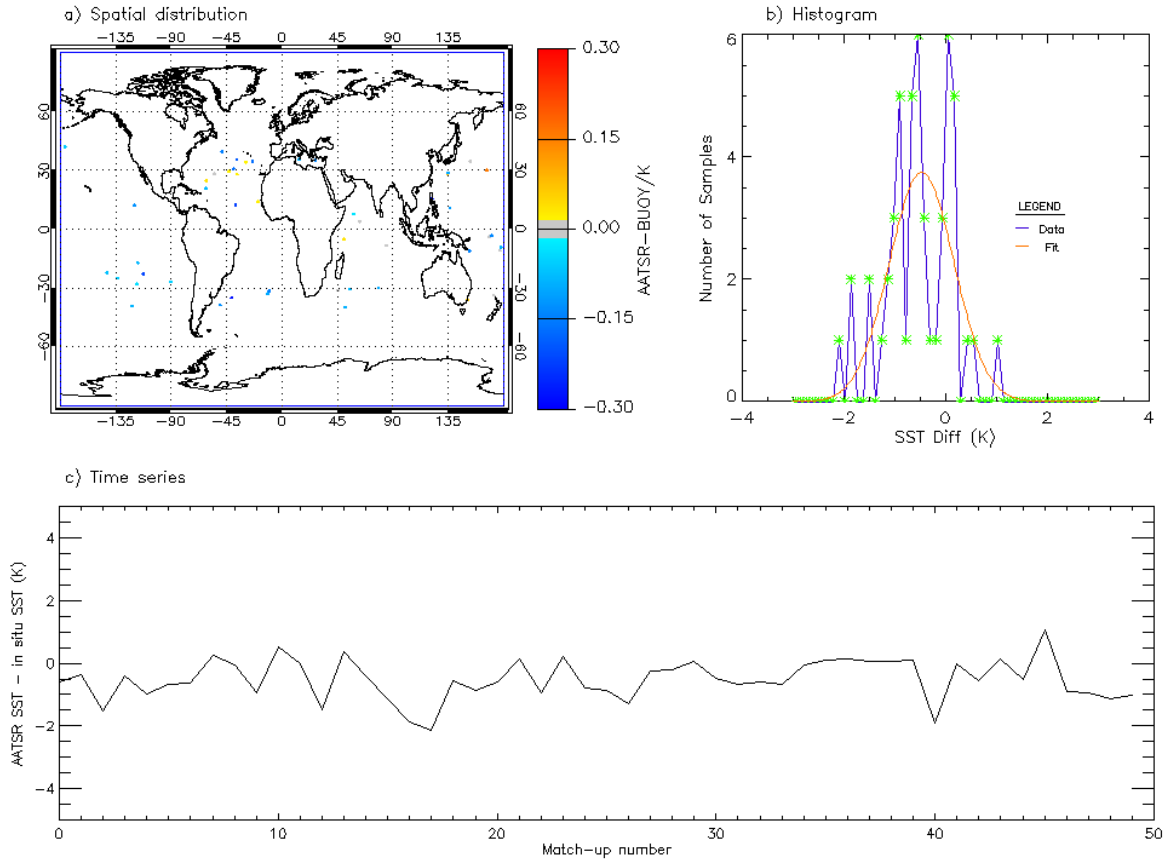

Figure 3-21: Spatial distribution, histogram and time series of Case 4 match-ups, 2-channel retrieval, D-N < TL_2, wind speed > 6 m^{-1}

The statistics for the Case 4 match-ups are given in Table 3-8. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-8: Statistics for Case 4 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	51	-0.518	0.65	-0.556	0.66
Moored only	3	-6.445	9.63	-1.648	-
Ships only	23	-1.149	1.02	-1.015	1.07
TTP* only	3	-0.071	0.18	-0.150	0.30

*TTP = TAO/TRITON/PIRATA moored buoys

3.3.6 Case 5: 2-channel retrieval, D-N > TU_2, wind speed < 6 m^{-1}

Figure 3-22 shows a) the spatial distribution of Case 5 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between AATSR and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

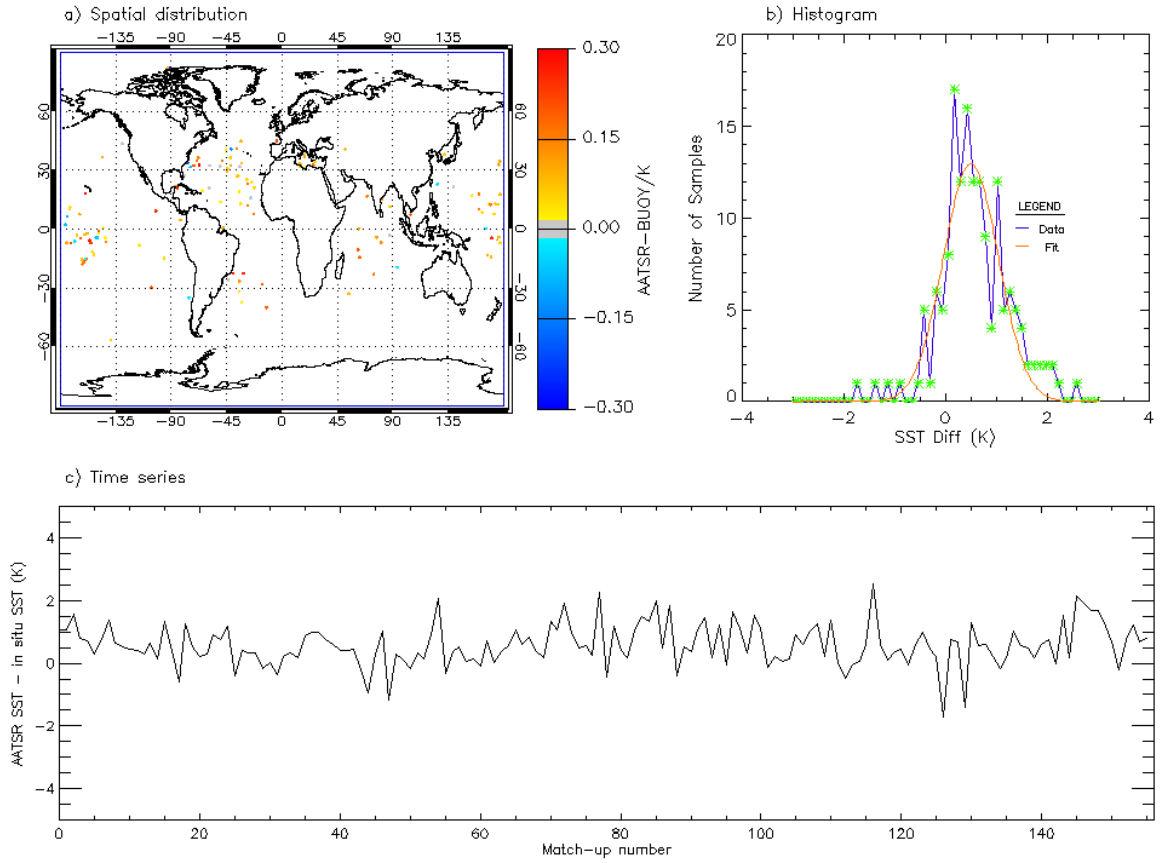

Figure 3-22: Spatial distribution, histogram and time series of Case 5 match-ups, 2-channel retrieval, D-N > TU_2, wind speed < 6 m^{-1}

The statistics for the Case 5 match-ups are given in Table 3-9. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-9: Statistics for Case 5 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	159	+0.586	0.68	+0.525	0.64
Moored only	27	+0.542	0.95	+0.772	0.99
Ships only	55	+0.456	1.71	+0.630	1.54
TTP* only	13	+0.216	0.65	+0.110	0.69

*TTP = TAO/TRITON/PIRATA moored buoys

3.3.7 Case 6: 2-channel retrieval, D-N > TU_2, wind speed > 6 m^{-1}

Figure 3-23 shows a) the spatial distribution of Case 6 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between AATSR and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

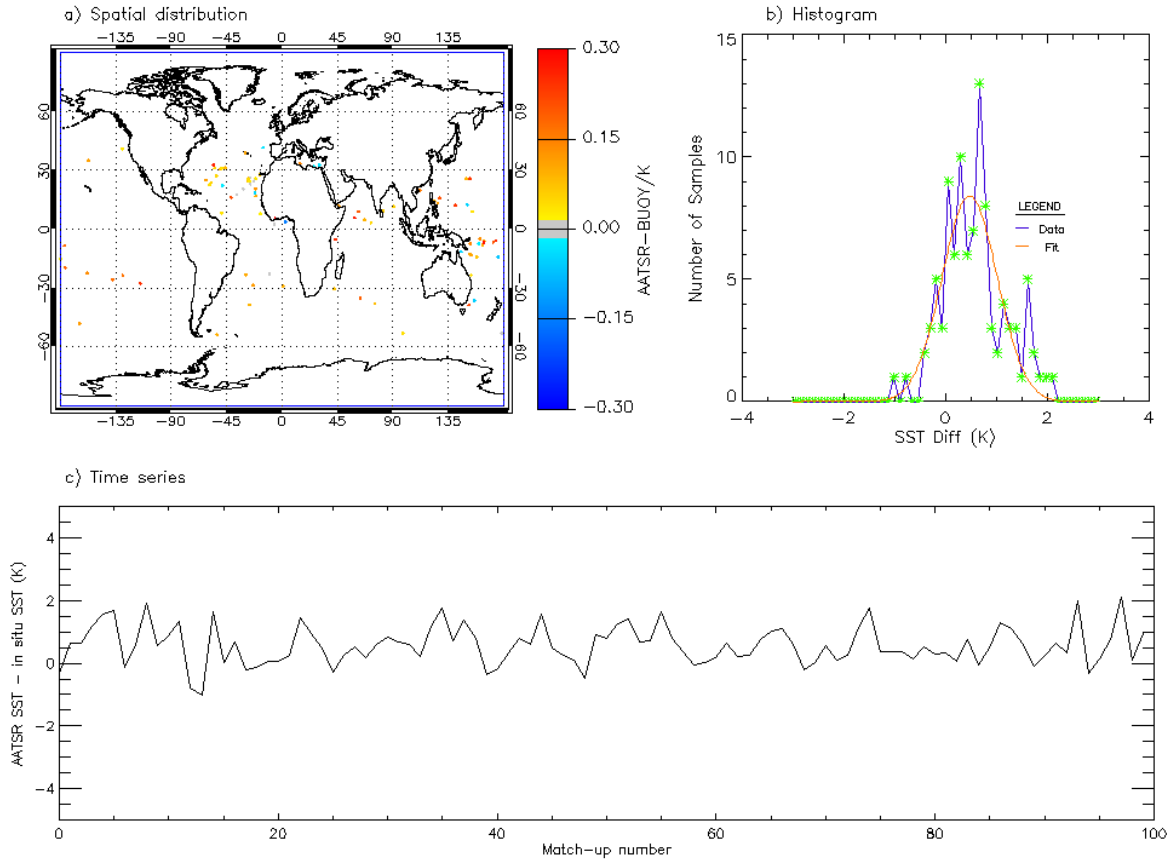

Figure 3-23: Spatial distribution, histogram and time series of Case 6 match-ups, 2-channel retrieval, D-N > TU_2, wind speed > 6 m^{-1}

The statistics for the Case 6 match-ups are given in Table 3-10. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-10: Statistics for Case 6 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	102	+0.571	0.62	+0.571	0.63
Moored only	11	+0.657	0.58	+0.410	0.63
Ships only	66	+0.464	1.53	+0.292	1.27
TTP* only	4	+0.467	0.41	+0.495	0.45

*TTP = TAO/TRITON/PIRATA moored buoys

3.3.8 Case 7: 3-channel retrieval, $TL_3 < D\text{-}N < TU_3$, wind speed < 6 m^{-1}

Figure 3-24 shows a) the spatial distribution of Case 7 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between AATSR and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

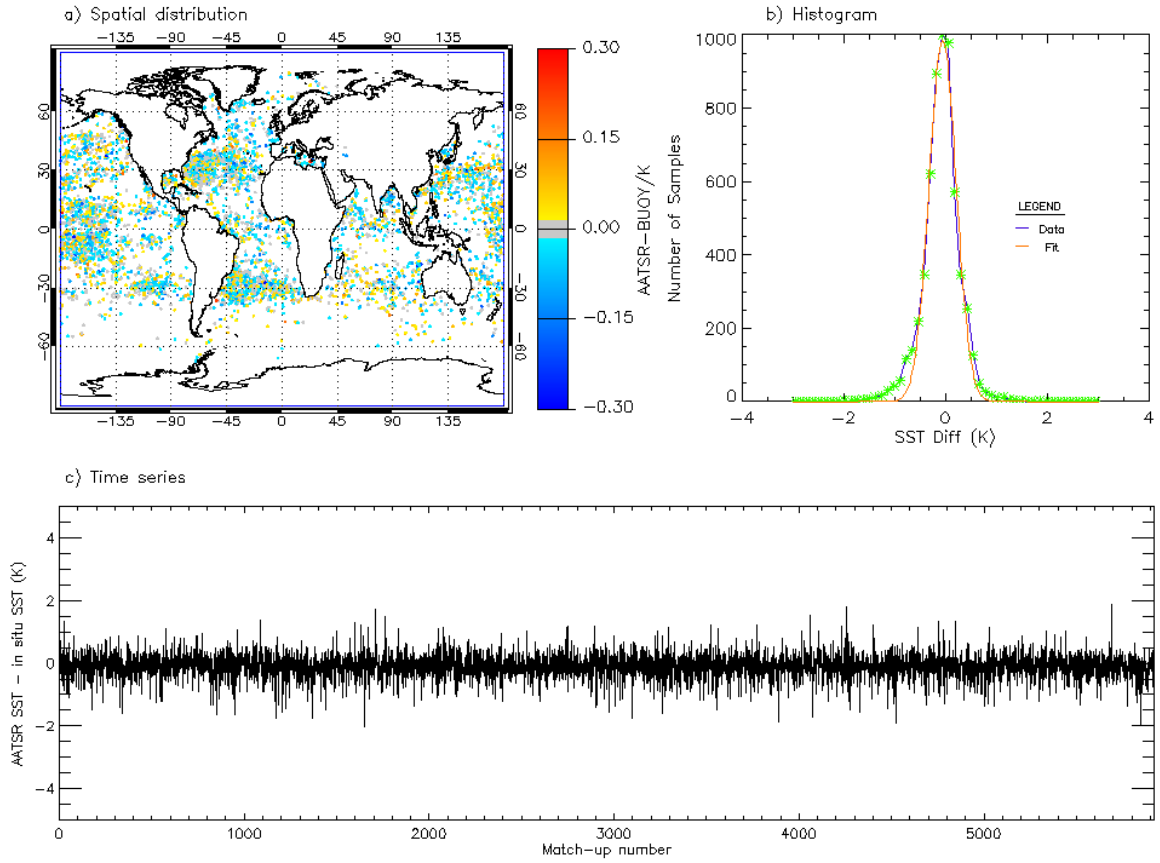

Figure 3-24: Spatial distribution, histogram and time series of Case 7 match-ups, 3-channel retrieval, $TL_3 < D\text{-}N < TU_3$, wind speed < 6 m^{-1}

The statistics for the Case 7 match-ups are given in Table 3-11. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-11: Statistics for Case 7 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	5975	-0.084	0.36	+0.061	0.32
Moored only	878	-0.078	0.55	-0.119	0.40
Ships only	1891	-0.165	1.38	-0.228	1.09
TTP* only	338	-0.106	0.27	-0.075	0.27

*TTP = TAO/TRITON/PIRATA moored buoys

3.3.9 Case 8: 3-channel retrieval, $TL_3 < D\text{-}N < TU_3$, wind speed > 6 m^{-1}

Figure 3-25 shows a) the spatial distribution of Case 8 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between AATSR and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

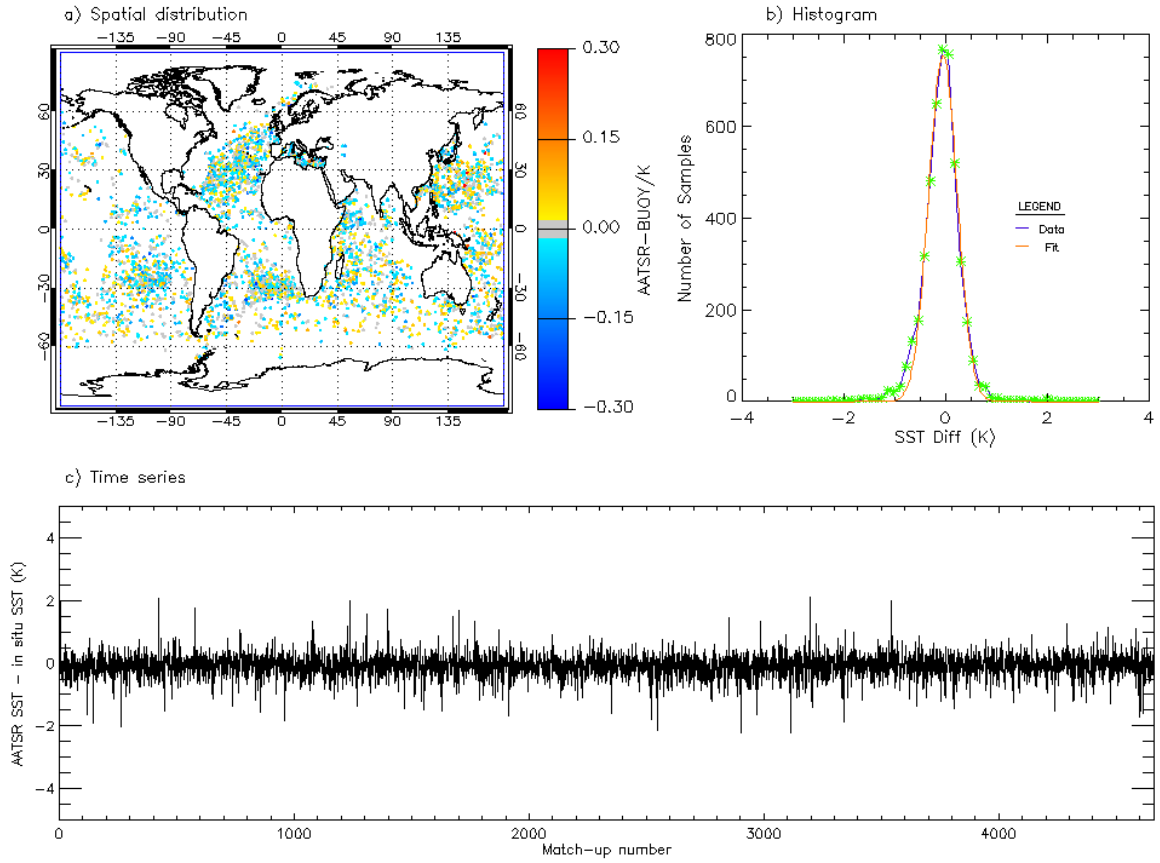

Figure 3-25: Spatial distribution, histogram and time series of Case 8 match-ups, 3-channel retrieval, $TL_3 < D\text{-}N < TU_3$, wind speed > 6 m^{-1}

The statistics for the Case 8 match-ups are given in Table 3-12. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-12: Statistics for Case 8 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	4707	-0.080	0.36	-0.061	0.32
Moored only	237	-0.003	0.72	+0.015	0.46
Ships only	1829	-0.078	1.44	-0.171	1.13
TTP* only	105	-0.145	0.27	-0.119	0.26

*TTP = TAO/TRITON/PIRATA moored buoys

3.3.10 Case 9: 3-channel retrieval, D-N < TL_3, wind speed < 6 m^{-1}

Figure 3-26 shows a) the spatial distribution of Case 9 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between AATSR and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

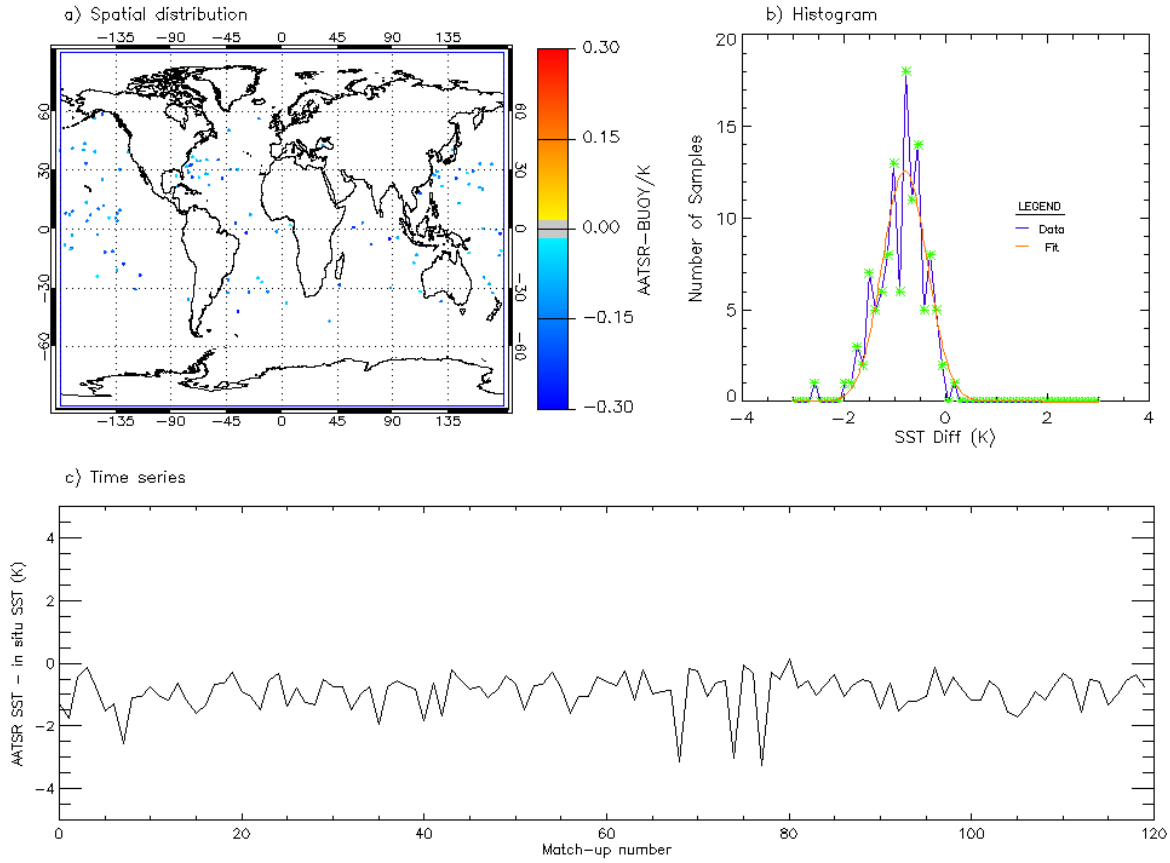

Figure 3-26: Spatial distribution, histogram and time series of Case 9 match-ups, 3-channel retrieval, D-N < TL_3, wind speed < 6 m^{-1}

The statistics for the Case 9 match-ups are given below. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-13: Statistics for Case 9 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	122	-0.924	0.58	-0.780	0.47
Moored only	83	-0.582	0.74	-0.648	0.71
Ships only	61	-1.054	1.33	-0.935	1.22
TTP* only	9	-0.795	0.29	-0.750	0.31

*TTP = TAO/TRITON/PIRATA moored buoys

3.3.11 Case 10: 3-channel retrieval, D-N < TL_3, wind speed > 6 m^{-1}

Figure 3-27 shows a) the spatial distribution of Case 10 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between AATSR and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

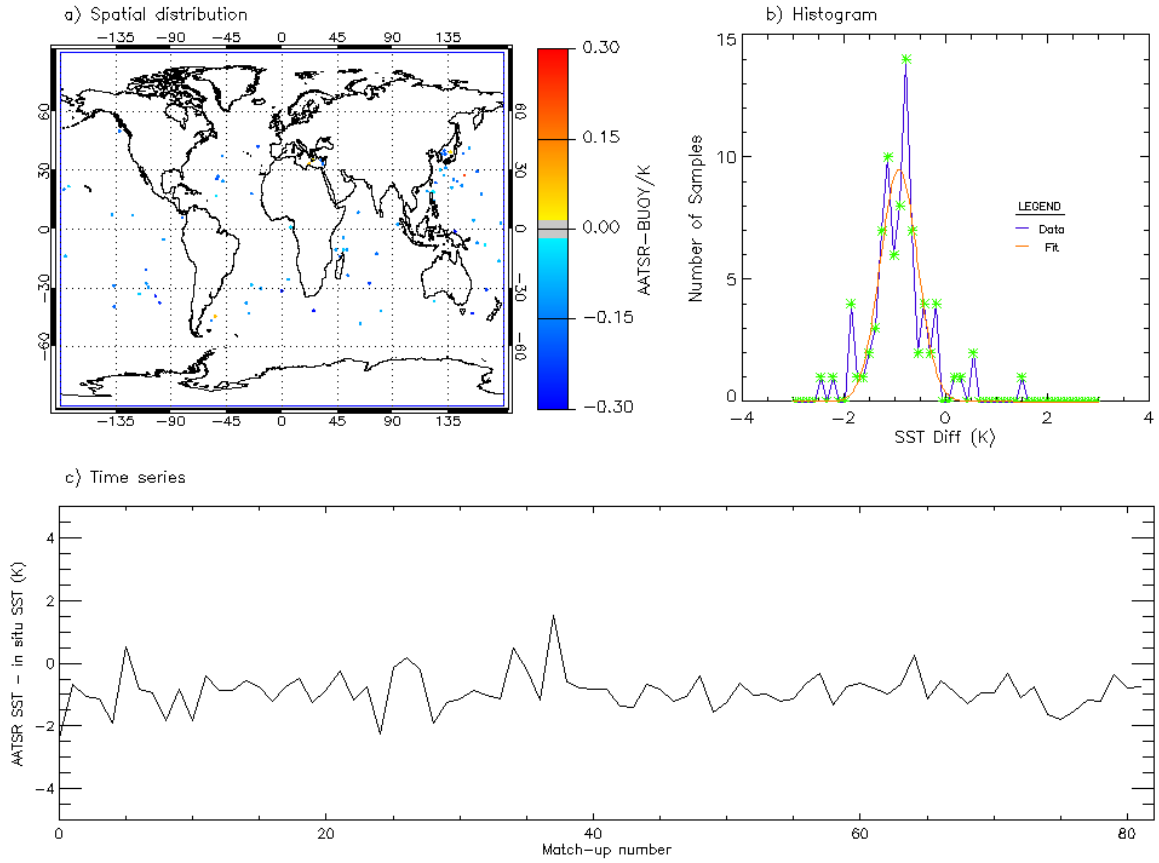

Figure 3-27: Spatial distribution, histogram and time series of Case 10 match-ups, 3-channel retrieval, D-N < TL_3, wind speed > 6 m^{-1}

The statistics for the Case 10 match-ups are given in Table 3-14. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-14: Statistics for Case 10 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	85	-0.888	0.60	-0.865	0.51
Moored only	5	-0.604	0.85	-0.692	0.90
Ships only	37	-1.162	1.24	-0.980	1.00
TTP* only	4	-0.883	0.30	-0.936	0.34

*TTP = TAO/TRITON/PIRATA moored buoys

3.3.12 Case 11: 3-channel retrieval, D-N > TU_3, wind speed < 6 m^{-1}

Figure 3-28 shows a) the spatial distribution of Case 11 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between AATSR and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

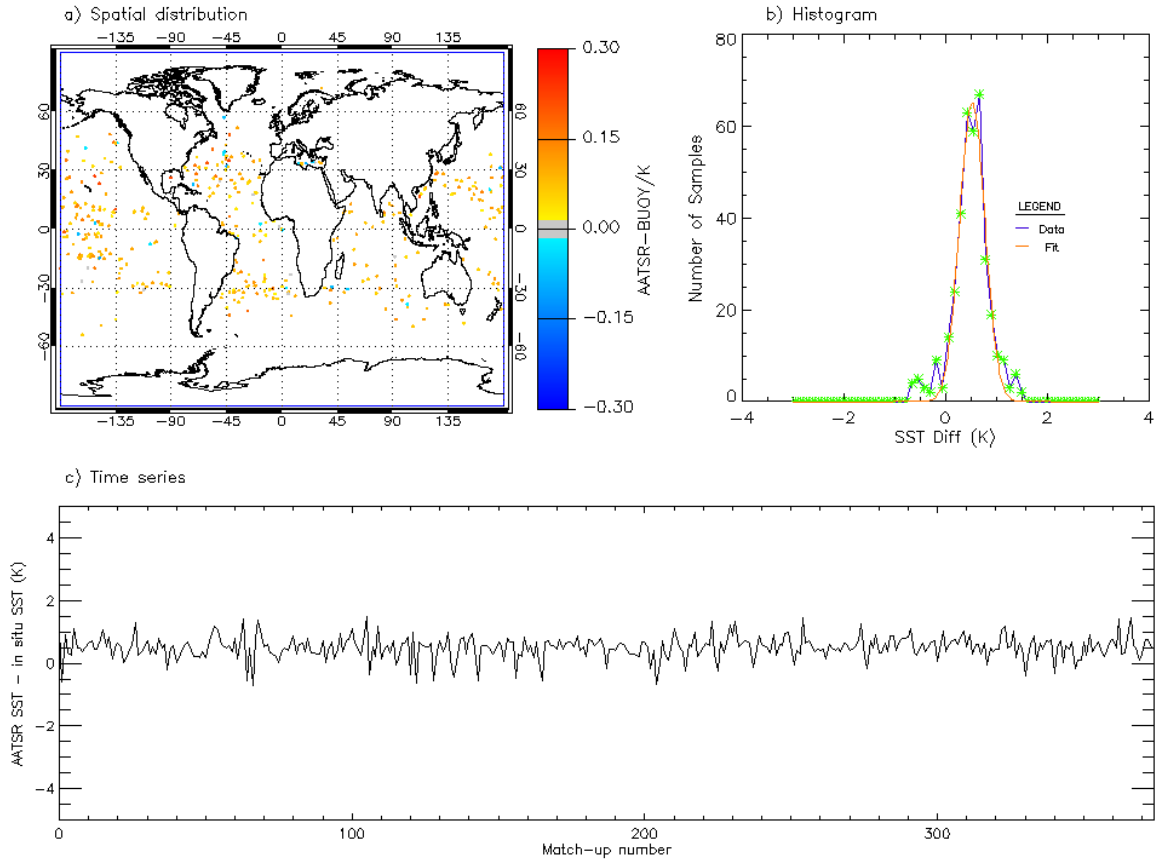

Figure 3-28: Spatial distribution, histogram and time series of Case 11 match-ups, 3-channel retrieval, D-N > TU_3, wind speed < 6 m^{-1}

The statistics for the Case 11 match-ups are given in Table 3-15. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-15: Statistics for Case 11 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	382	+0.504	0.36	+0.524	0.32
Moored only	27	+0.546	0.45	+0.493	0.32
Ships only	107	+0.129	1.70	+0.371	1.35
TTP* only	24	+0.416	0.40	+0.460	0.37

*TTP = TAO/TRITON/PIRATA moored buoys

3.3.13 Case 12: 3-channel retrieval, D-N > TU_3, wind speed > 6 m^{-1}

Figure 3-29 shows a) the spatial distribution of Case 12 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between AATSR and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

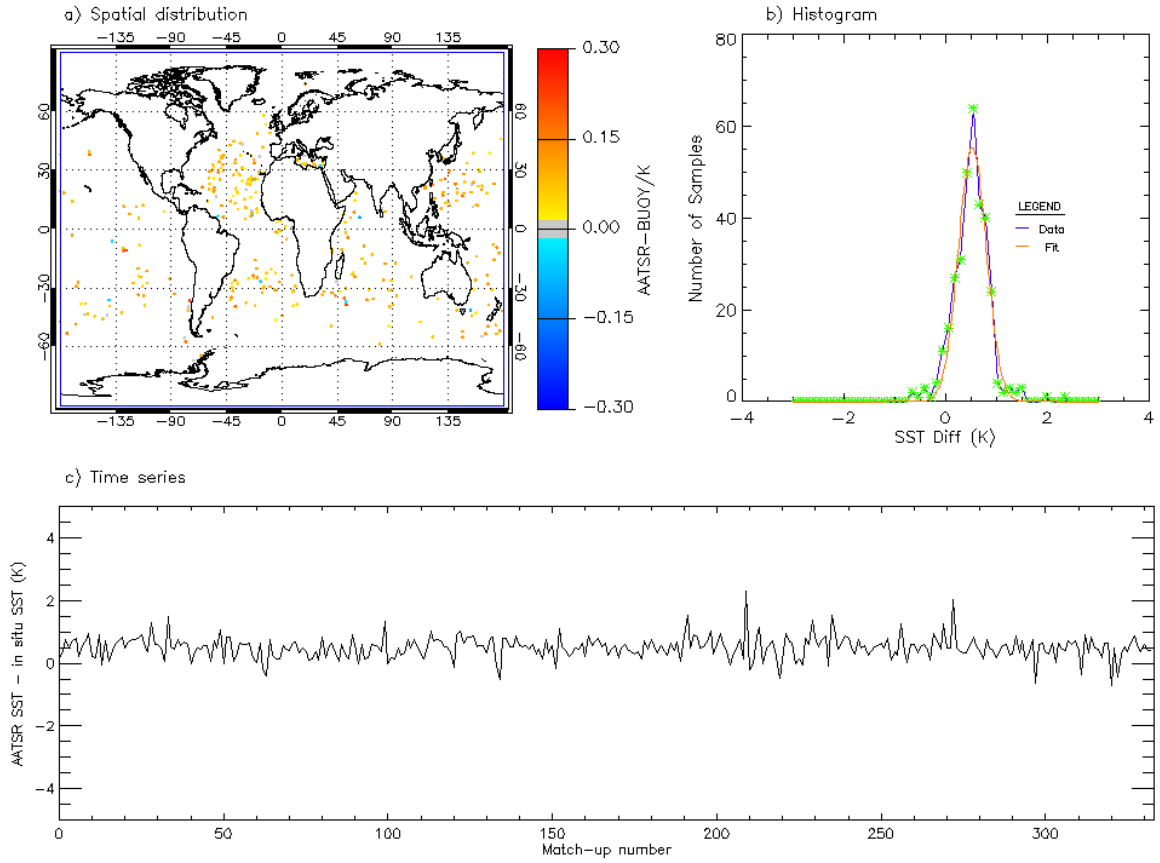

Figure 3-29: Spatial distribution, histogram and time series of Case 12 match-ups, 3-channel retrieval, D-N < TU_3, wind speed > 6 m^{-1}

The statistics for the Case 12 match-ups are given in Table 3-16. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-16: Statistics for Case 12 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	336	+0.504	0.35	+0.524	0.31
Moored only	16	-1.477	5.71	+0.560	0.48
Ships only	137	+0.469	1.29	+0.269	1.00
TTP* only	8	+0.493	0.24	+0.585	0.26

*TTP = TAO/TRITON/PIRATA moored buoys

3.3.14 Summary of the Analysis

Table 3-17 summarises the match-up statistics for all 12 cases. Additional match-up statistics are provided in tables 3-18 to 3-23, where the wind speed dependency has been removed. Inspection of tables 3-17 to 3-23 highlights the following:

- The wind speed dependence observed in analysis of the Medspiration database [AD2] is not apparent.
- If wind speed dependence is ignored, then the calculated biases and standard deviations are very similar to those calculated for Medspiration.
- The robust statistics for cases 1, 2, 7 and 8 (which are uncontaminated retrievals) are very similar to the non-robust statistics.

The AATSR SSTs are skin SSTs whereas the in situ data from the MDB are measured below the surface. If we ignore any effects of diurnal warming, we may consider the in situ data to represent the sub-skin SST. Since this has been shown on average to be 0.17 K warmer than the skin SST (AD5), this must introduce an additional negative bias in the value of the difference between satellite and in situ observations. To remove this artefact from the error statistics, an adjustment of + 0.17 K should be added to all biases when converting tables 3-17 to 3-23 into the SSES bias values.

Table 3-17: Summary of validation statistics for all stratification cases

Data Set		Statistics				
		Number	Mean (ºC)	Sigma (ºC)	Median (ºC)	Robust Sigma (ºC)
Case 1	Drifters only	4394	+0.022	0.38	+0.030	0.33
	Moored only	708	-0.131	0.64	-0.129	0.54
	Ships only	1742	-0.052	1.39	-0.141	1.17
	TTP* only	184	+0.010	0.32	+0.010	0.31
Case 2	Drifters only	3907	+0.034	0.36	+0.022	0.32
	Moored only	176	-0.201	2.11	+0.059	0.58
	Ships only	1625	-0.167	1.38	-0.180	1.16
	TTP* only	51	+0.033	0.30	+0.022	0.30
Case 3	Drifters only	110	-0.625	0.70	-0.580	0.72
	Moored only	27	-0.526	0.76	-0.430	0.79
	Ships only	46	-0.952	1.49	-0.670	1.49
	TTP* only	8	-0.669	0.83	-0.495	0.85
Case 4	Drifters only	51	-0.518	0.65	-0.556	0.66
	Moored only	3	-6.445	9.63	-1.648	-
	Ships only	23	-1.149	1.02	-1.015	1.07
	TTP* only	3	-0.071	0.18	-0.150	0.30
Case 5	Drifters only	159	+0.586	0.68	+0.525	0.64
	Moored only	27	+0.542	0.95	+0.772	0.99
	Ships only	55	+0.456	1.71	+0.630	1.54
	TTP* only	13	+0.216	0.65	+0.110	0.69
Case 6	Drifters only	102	+0.571	0.62	+0.571	0.63
	Moored only	11	+0.657	0.58	+0.410	0.63
	Ships only	66	+0.464	1.53	+0.292	1.27
	TTP* only	4	+0.467	0.41	+0.495	0.45
Case 7	Drifters only	5975	-0.084	0.36	+0.061	0.32
	Moored only	878	-0.078	0.55	-0.119	0.40
	Ships only	1891	-0.165	1.38	-0.228	1.09
	TTP* only	338	-0.106	0.27	-0.075	0.27
Case 8	Drifters only	4707	-0.080	0.36	-0.061	0.32
	Moored only	237	-0.003	0.72	+0.015	0.46
	Ships only	1829	-0.078	1.44	-0.171	1.13
	TTP* only	105	-0.145	0.27	-0.119	0.26
Case 9	Drifters only	122	-0.924	0.58	-0.780	0.47
	Moored only	83	-0.582	0.74	-0.648	0.71
	Ships only	61	-1.054	1.33	-0.935	1.22
	TTP* only	9	-0.795	0.29	-0.750	0.31

Data Set		Statistics				
		Number	Mean (ºC)	Sigma (ºC)	Median (ºC)	Robust Sigma (ºC)
Case 10	Drifters only	85	-0.888	0.60	-0.865	0.51
	Moored only	5	-0.604	0.85	-0.692	0.90
	Ships only	37	-1.162	1.24	-0.980	1.00
	TTP* only	4	-0.883	0.30	-0.936	0.34
Case 11	Drifters only	382	+0.504	0.36	+0.524	0.32
	Moored only	27	+0.546	0.45	+0.493	0.32
	Ships only	107	+0.129	1.70	+0.371	1.35
	TTP* only	24	+0.416	0.40	+0.460	0.37
Case 12	Drifters only	336	+0.504	0.35	+0.524	0.31
	Moored only	16	-1.477	5.71	+0.560	0.48
	Ships only	137	+0.469	1.29	+0.269	1.00
	TTP* only	8	+0.493	0.24	+0.585	0.26

*TTP = TAO/TRITON/PIRATA moored buoys

Table 3-18: Statistics for 2-channel retrieval, TL_2 < D-N < TU_2 (combining cases 1 and 2)

Dataset	Statistics				
	Number	Mean (°C)	Sigma (°C)	Median (°C)	Robust Sigma(°C)
Drifters only	8301	+0.025	0.37	+0.028	0.32
Moored only	884	-0.106	0.76	-0.090	0.56
Ships only	3367	-0.109	1.38	-0.162	1.16
TTP* only	235	-0.005	0.33	+0.020	0.31

*TTP = TAO/TRITON/PIRATA moored buoys

Table 3-19: Statistics for 2-channel retrieval, D-N < TL_2 (combining cases 3 and 4)

Dataset	Statistics				
	Number	Mean (°C)	Sigma (°C)	Median (°C)	Robust Sigma(°C)
Drifters only	161	-0.609	0.72	-0.579	0.71
Moored only	30	-0.553	0.77	-0.430	0.80
Ships only	69	-1.015	1.35	-0.939	1.35
TTP* only	11	-0.506	0.75	-0.202	0.68

*TTP = TAO/TRITON/PIRATA moored buoys

Table 3-20: Statistics for 2-channel retrieval, D-N > TU_2 (combining cases 5 and 6)

Dataset	Statistics				
	Number	Mean (°C)	Sigma (°C)	Median (°C)	Robust Sigma(°C)
Drifters only	261	+0.580	0.65	+0.540	0.64
Moored only	38	+0.575	0.86	+0.645	0.87
Ships only	121	+0.512	1.70	+0.451	1.43
TTP* only	17	+0.276	0.60	+0.212	0.63

*TTP = TAO/TRITON/PIRATA moored buoys

Table 3-21: Statistics for 3-channel retrieval, TL_3 < D-N < TU_3 (combining cases 7 and 8)

Dataset	Statistics				
	Number	Mean (°C)	Sigma (°C)	Median (°C)	Robust Sigma(°C)
Drifters only	10682	-0.082	0.36	-0.061	0.32
Moored only	1115	-0.055	0.62	-0.091	0.41
Ships only	3720	-0.114	1.43	-0.195	1.12
TTP* only	443	-0.116	0.27	-0.088	0.27

*TTP = TAO/TRITON/PIRATA moored buoys

Table 3-22: Statistics for 3-channel retrieval, D-N < TL_3 (combining cases 9 and 10)

Dataset	Statistics				
	Number	Mean (°C)	Sigma (°C)	Median (°C)	Robust Sigma(°C)
Drifters only	207	-0.895	0.62	-0.819	0.49
Moored only	88	-0.583	0.74	-0.654	0.71
Ships only	98	-1.095	1.29	-0.935	1.14
TTP* only	13	-0.822	0.28	-0.901	0.31

*TTP = TAO/TRITON/PIRATA moored buoys

Table 3-23: Statistics for 3-channel retrieval, D-N > TU_3 (combining cases 11 and 12)

Dataset	Statistics				
	Number	Mean (°C)	Sigma (°C)	Median (°C)	Robust Sigma(°C)
Drifters only	718	+0.504	0.37	+0.521	0.32
Moored only	43	+0.375	1.30	+0.548	0.36
Ships only	244	+0.320	1.49	+0.305	1.16
TTP* only	32	+0.435	0.36	+0.475	0.32

*TTP = TAO/TRITON/PIRATA moored buoys

3.4 ATSR-2

All three sensors in the (A)ATSR series are similar, so it is reasonable to assume that the known error sources are similar for all three instruments. Therefore, the SSES scheme for ATSR-2 is based on that derived for AATSR, and involves a 12-fold stratification of the MDB, based on the D-N SST difference and wind speed. This section summarises the calculation of the D-N thresholds for ATSR-2, analysis of the ATSR-2 MDB and determination of the ATSR-2 SSES.

3.4.1 Calculation of D-N thresholds

The ATSR-2 D-N thresholds are derived using the same method developed for AATSR, from analysis of relatively aerosol free months October 1997 to March 1998 for the Caribbean and the Bay of Biscay. Only one year has been analysed so far to allow an initial applicability test of AATSR SSES methodology to ATSR-2. The histograms of the D-N differences are shown in Figure 3-30, and a summary of the thresholds is given in Table 3-24.

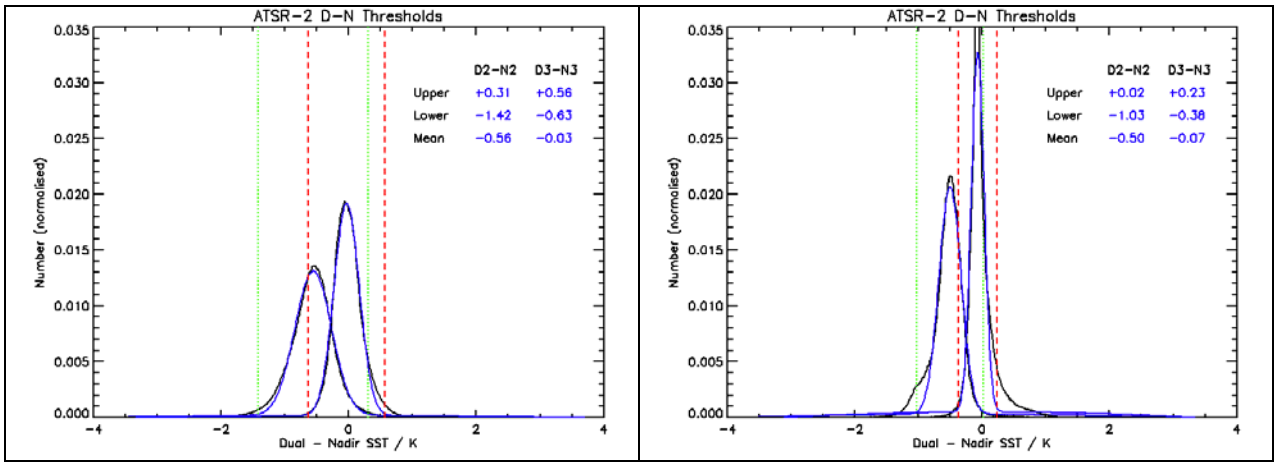

Figure 3-30: Histogram of D-N differences for D2-N2 and D3-N3 SST retrievals at full resolution for relatively aerosol-clear months of October 1997 to March 1998 for the Caribbean (left) and the Bay of Biscay (right). The 3-sigma limits for D2-N2 are indicated by the green dotted lines, and the 3-sigma limits for D3-N3 are indicated by the red dashed lines.

	D2-N2		D3-N3	
Region	**Upper**	**Lower**	**Upper**	**Lower**
Caribbean 10/97 to 03/98	+0.31	-1.42	+0.56	-0.63
Biscay 10/97 to 03/98	+0.02	-1.03	+0.23	-0.38

Table 3-24: Summary of D-N thresholds

For the global threshold, a mean value is taken and a standard error is applied. The final ATSR-2 D-N thresholds are:

- TU_2 = + 0.17 ± 0.21 K
- TL_2 = - 1.23 ± 0.27 K
- TU_3 = + 0.40 ± 0.23 K
- TL_3 = - 0.51 ± 0.18 K

The histograms and calculated thresholds are quite similar to those observed for AATSR, with a positive shift in the 2-channel thresholds that may be due to the observed 12-micron offset. The variances for ATSR-2 are notably larger to those calculated for AATSR, the reasons for which are not yet understood.

3.4.2 Analysis of MDB

A basic analysis of the ATSR-2 MDB was carried out using the method derived for AATSR and the ATSR-2 D-N thresholds detailed section 3.4.1. As for AATSR, a ± 3 sigma filter is applied before calculating the mean bias and standard deviation to remove any remaining outliers that would otherwise overly affect the statistics. Both robust and non-robust statistics are reported.

3.4.3 Case 1: 2-channel retrieval; TL_2 < D-N < TU_2, wind speed < 6 m^{-1}

Figure 3-31 shows (a) the spatial distribution of Case 1 match-ups, (b) the histogram of the match-ups (together with a fitted Gaussian), and (c) a time series of the differences between ATSR-2 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

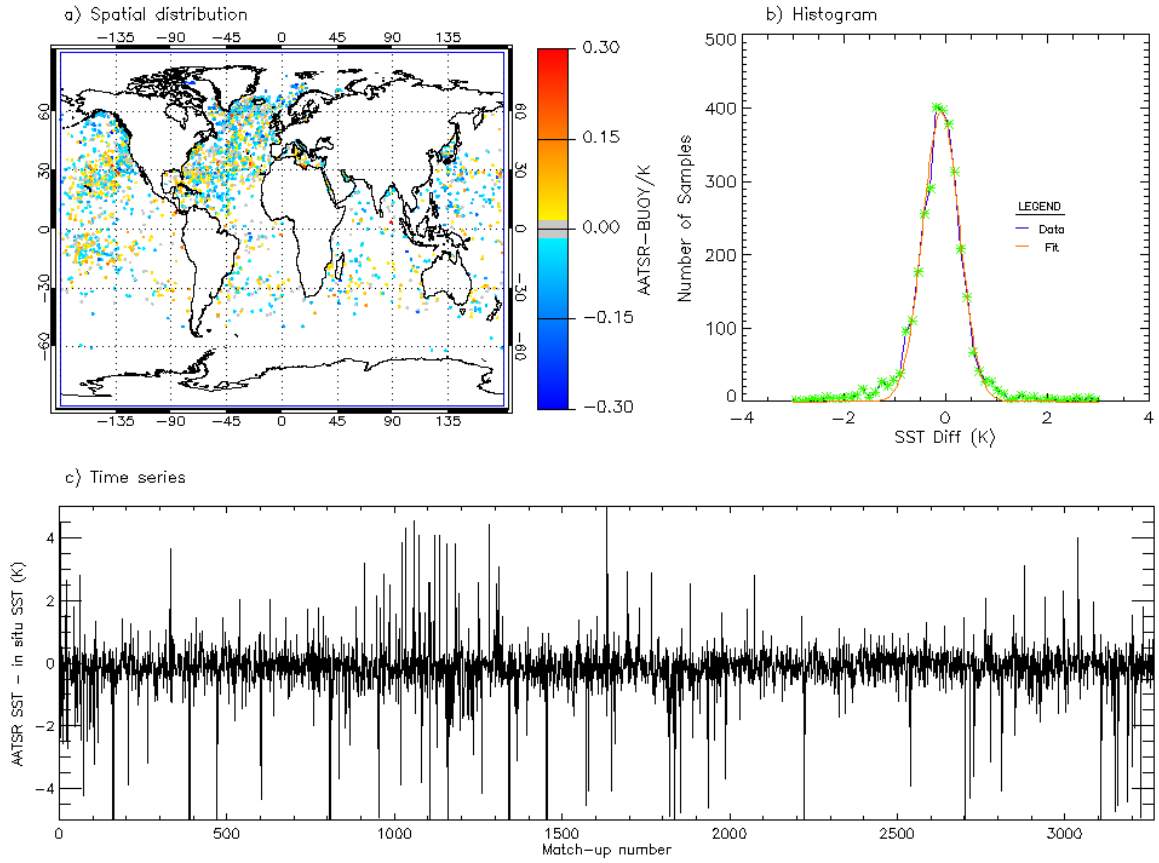

Figure 3-31: Spatial distribution, histogram and time series of Case 1 match-ups, 2-channel retrieval, TL_2 < D-N < TU_2, wind speed < 6 m^{-1}

The statistics for the Case 1 match-ups are given in Table 3-25. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-25: Statistics for Case 1 match-ups

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	3301	-0.151	0.81	-0.100	0.43
Moored only	2127	-0.056	0.63	-0.069	0.51
Ships only	10987	-0.159	1.48	-0.199	1.21
TTP* only	492	-0.125	0.34	-0.120	0.31

*TTP = TAO/TRITON/PIRATA moored buoys

3.4.4 Case 2: 2-channel retrieval, $TL_2 < D\text{-}N < TU_2$, wind speed > 6 m^{-1}

Figure 3-32 shows a) the spatial distribution of Case 2 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between ATSR-2 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

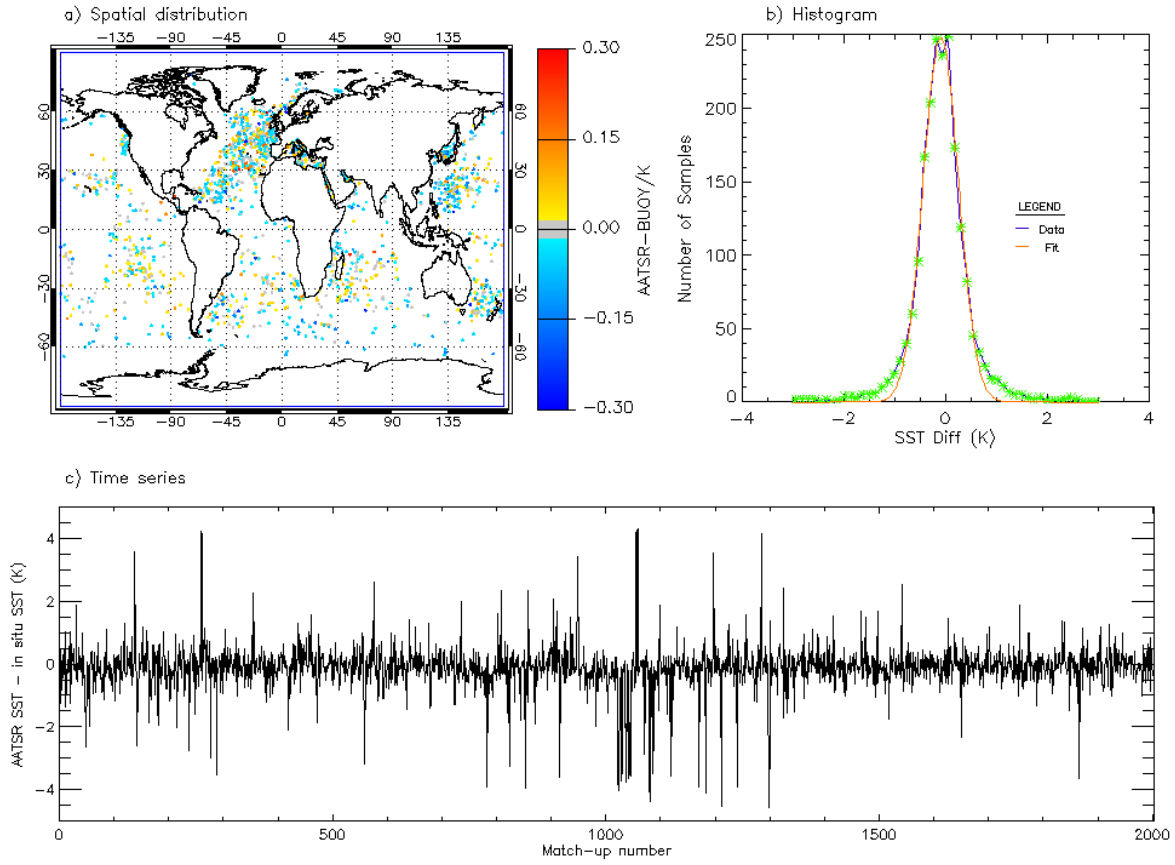

Figure 3-32: Spatial distribution, histogram and time series of Case 2 match-ups, 2-channel retrieval, $TL_2 < D\text{-}N < TU_2$, wind speed > 6 m^{-1}

The statistics for the Case 2 match-ups are given below. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-26: Statistics for Case 2 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	2033	-0.129	0.76	-0.100	0.43
Moored only	527	-0.097	0.73	-0.129	0.52
Ships only	8649	-0.216	1.42	-0.250	1.20
TTP* only	152	-0.133	0.30	-0.120	0.29

*TTP = TAO/TRITON/PIRATA moored buoys

3.4.5 Case 3: 2-channel retrieval, D-N < TL_2, wind speed < 6 m^{-1}

Figure 3-33 shows a) the spatial distribution of Case 3 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between ATSR-2 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

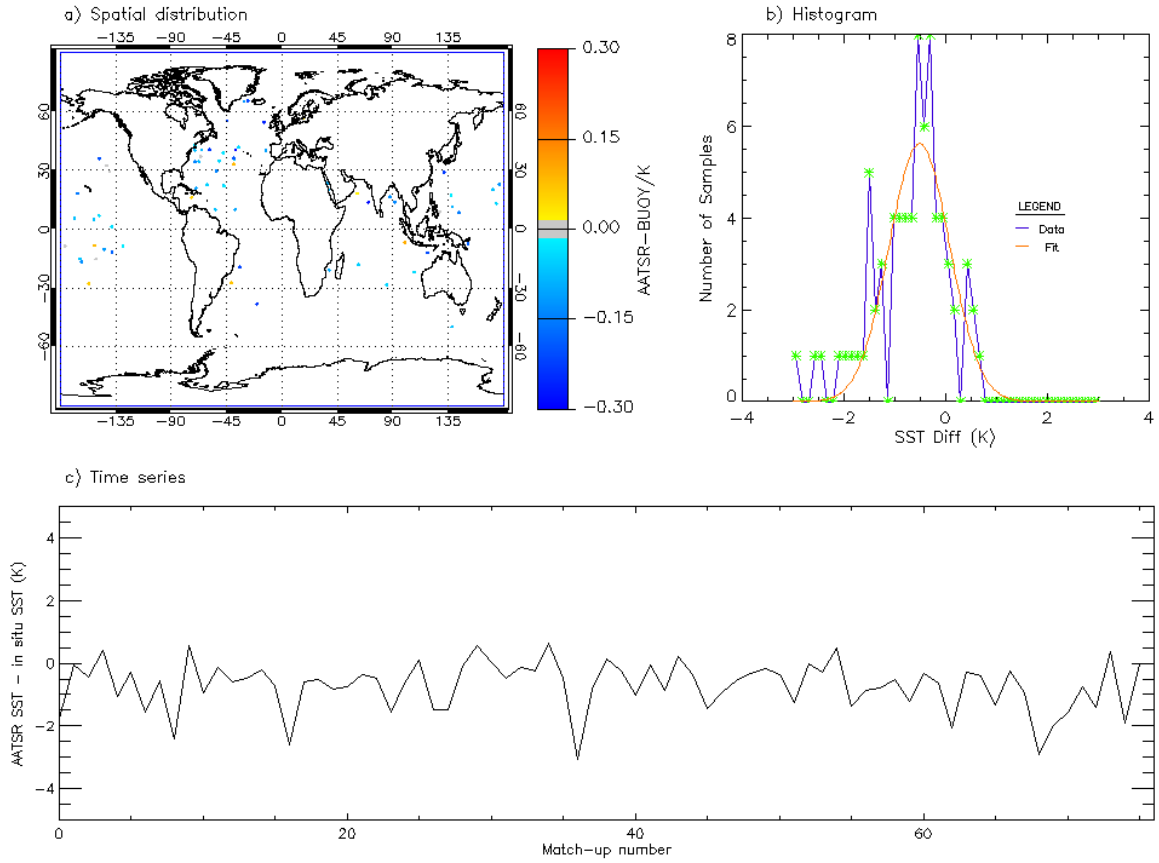

Figure 3-33: Spatial distribution, histogram and time series of Case 3 match-ups, 2-channel retrieval, D-N < TL_2, wind speed < 6 m^{-1}

The statistics for the Case 3 match-ups are given below. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-27: Statistics for Case 3 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	78	-0.708	0.79	-0.540	0.74
Moored only	55	-0.719	0.76	-0.771	0.78
Ships only	328	-0.626	1.58	-0.629	1.42
TTP* only	30	-0.749	0.69	-0.621	0.63

*TTP = TAO/TRITON/PIRATA moored buoys

3.4.6 Case 4: 2-channel retrieval, D-N < TL_2, wind speed > 6 m^{-1}

Figure 3-34 below shows a) the spatial distribution of Case 4 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between ATSR-2 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

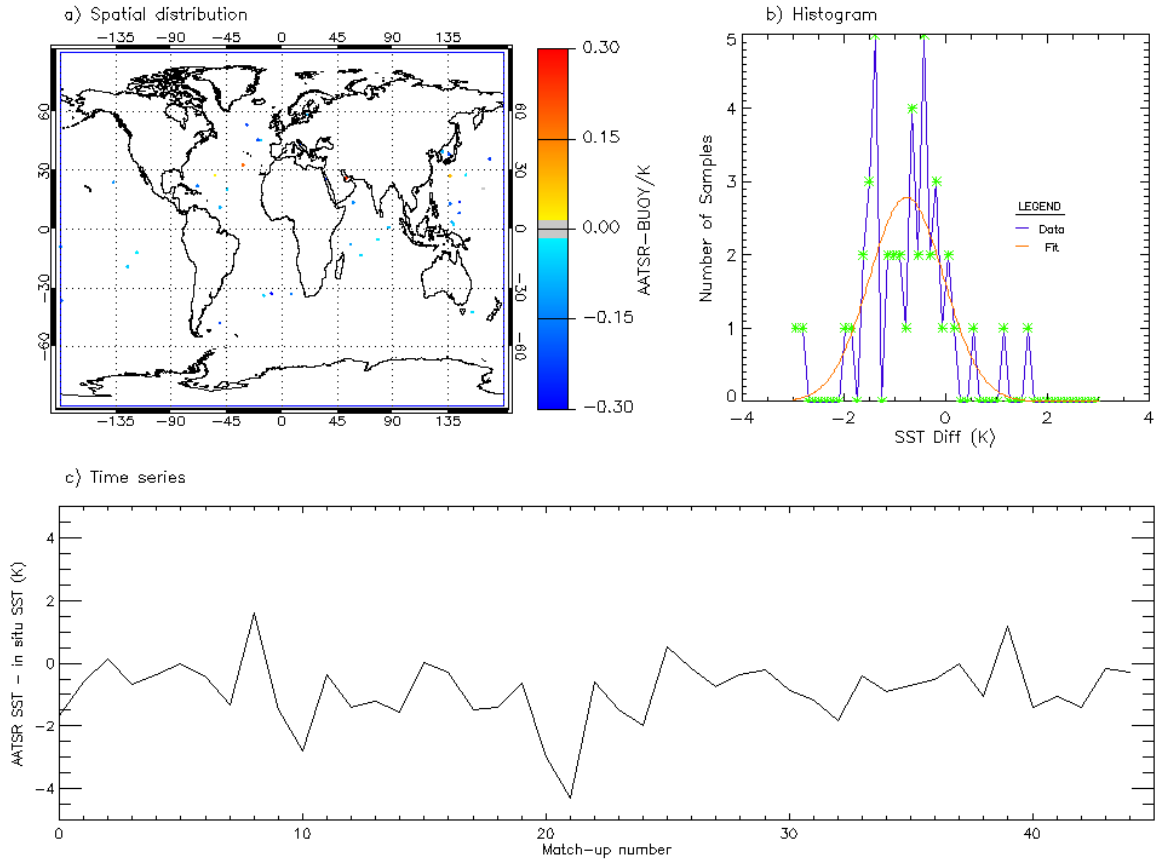

Figure 3-34: Spatial distribution, histogram and time series of Case 4 match-ups, 2-channel retrieval, D-N < TL_2, wind speed > 6 m^{-1}

The statistics for the Case 4 match-ups are given in Table 3-28. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-28: Statistics for Case 4 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	46	-0.863	1.01	-0.710	0.88
Moored only	4	-1.185	0.86	-1.439	0.97
Ships only	217	-0.654	1.40	-0.730	1.30
TTP* only	9	-0.418	0.37	-0.362	0.38

*TTP = TAO/TRITON/PIRATA moored buoys

3.4.7 Case 5: 2-channel retrieval, D-N > TU_2, wind speed < 6 m^{-1}

Figure 3-35 shows a) the spatial distribution of Case 5 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between ATSR-2 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

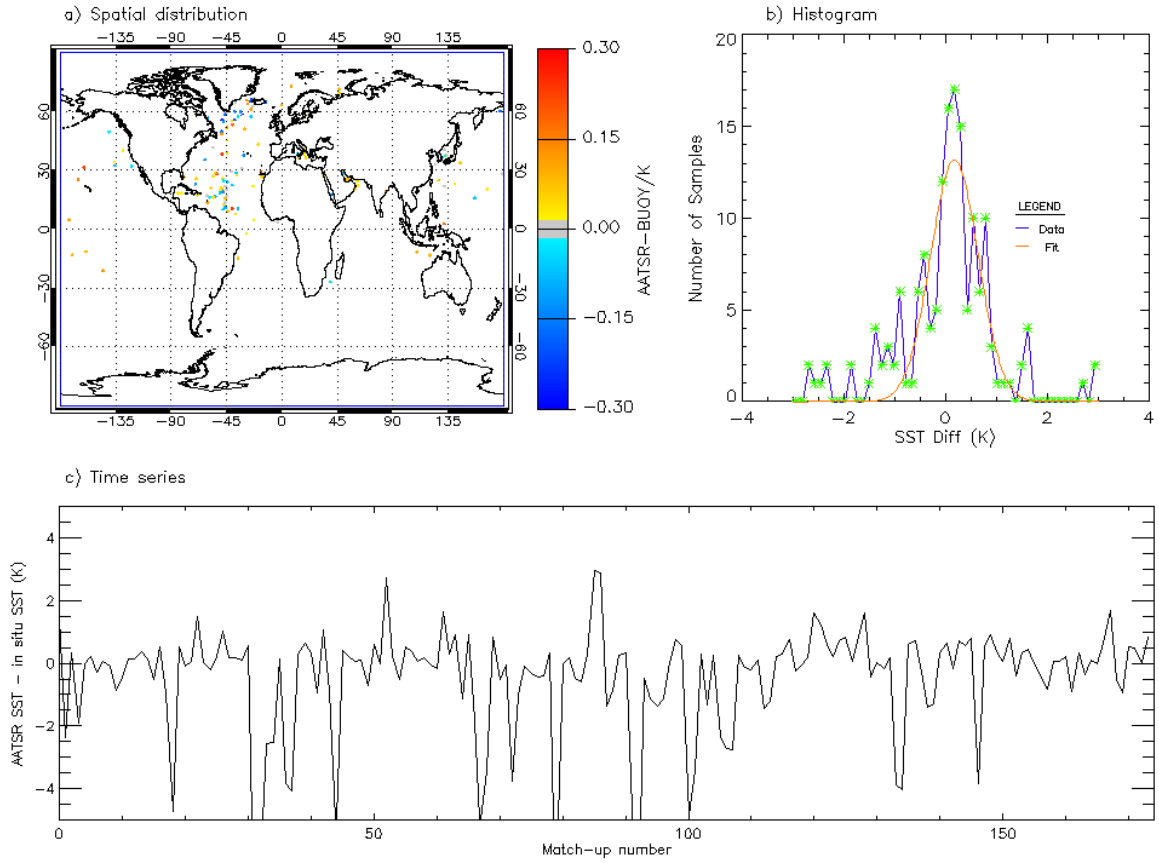

Figure 3-35: Spatial distribution, histogram and time series of Case 5 match-ups, 2-channel retrieval, D-N > TU_2, wind speed < 6 m^{-1}

The statistics for the Case 5 match-ups are given in Table 3-29. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-29: Statistics for Case 5 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	179	-0.488	1.85	+0.051	0.89
Moored only	106	-0.742	2.59	-0.059	1.16
Ships only	568	-0.188	2.16	-0.039	1.80
TTP* only	11	+0.682	0.54	+0.084	0.47

*TTP = TAO/TRITON/PIRATA moored buoys

3.4.8 Case 6: 2-channel retrieval, D-N > TU_2, wind speed > 6 m^{-1}

Figure 3-36 shows a) the spatial distribution of Case 6 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between ATSR-2 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

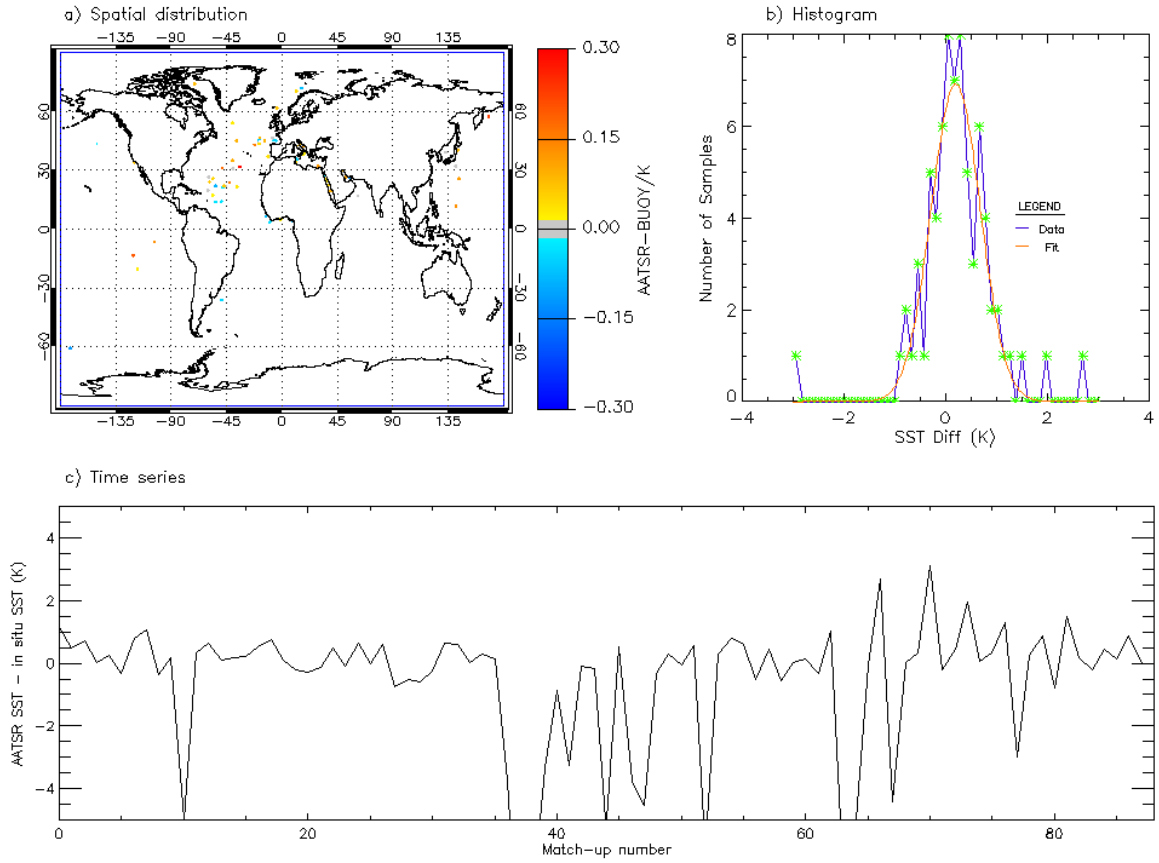

Figure 3-36: Spatial distribution, histogram and time series of Case 6 match-ups, 2-channel retrieval, D-N > TU_2, wind speed > 6 m^{-1}

The statistics for the Case 6 match-ups are given in Table 3-30. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-30: Statistics for Case 6 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	89	-0.545	2.17	+0.100	0.65
Moored only	14	-1.726	3.09	-0.100	1.27
Ships only	476	-0.034	1.85	+0.080	1.53
TTP* only	3	+0.516	0.58	+0.810	-

*TTP = TAO/TRITON/PIRATA moored buoys

3.4.9 Case 7: 3-channel retrieval, TL_3 < D-N < TU_3, wind speed < 6 m^{-1}

Figure 3-37 shows a) the spatial distribution of Case 7 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between ATSR-2 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

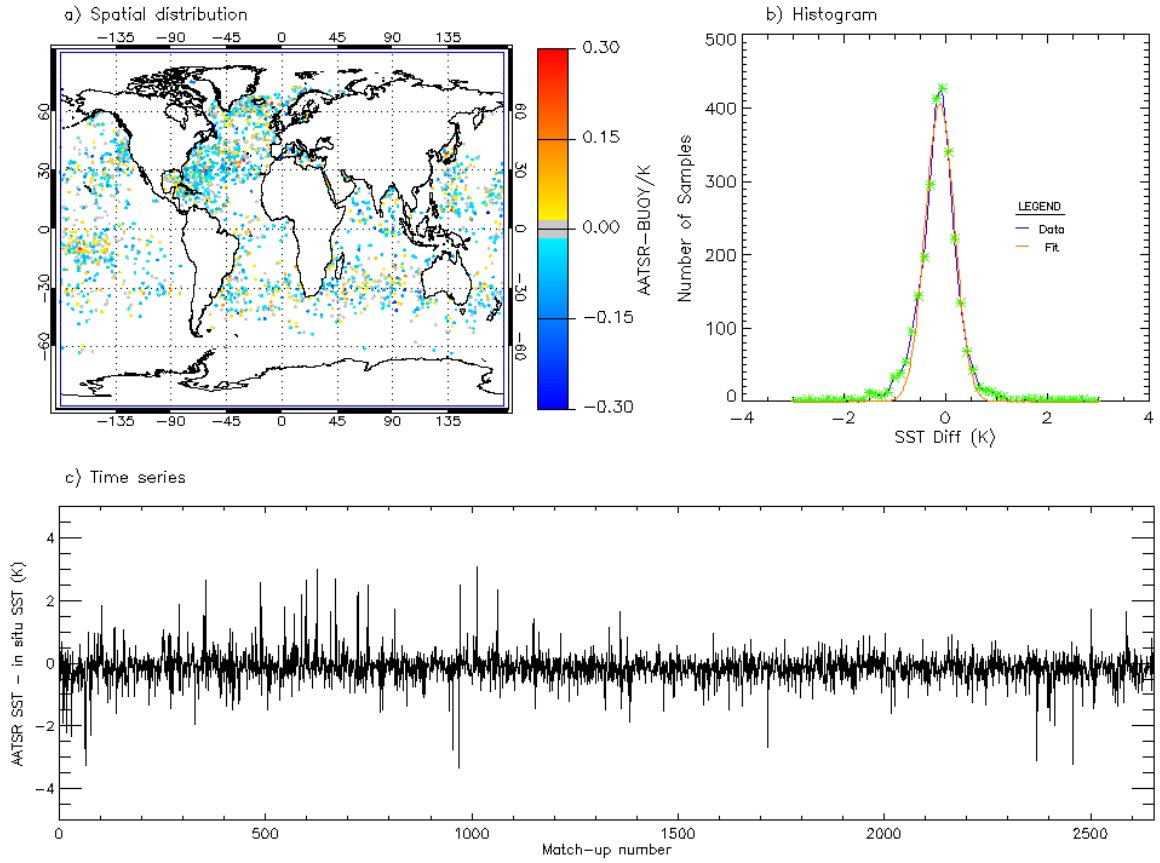

Figure 3-37: Spatial distribution, histogram and time series of Case 7 match-ups, 3-channel retrieval, TL_3 < D-N < TU_3, wind speed < 6 m^{-1}

The statistics for the Case 7 match-ups are given in Table 3-31. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-31: Statistics for Case 7 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	2698	-0.138	0.47	-0.121	0.35
Moored only	1829	-0.050	0.44	-0.040	0.40
Ships only	8809	-0.152	1.34	-0.170	1.09
TTP* only	437	-0.172	0.26	-0.160	0.25

*TTP = TAO/TRITON/PIRATA moored buoys

3.4.10 Case 8: 3-channel retrieval, $TL_3 < D\text{-}N < TU_3$, wind speed > 6 m^{-1}

Figure 3-38 shows a) the spatial distribution of Case 8 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between ATSR-2 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

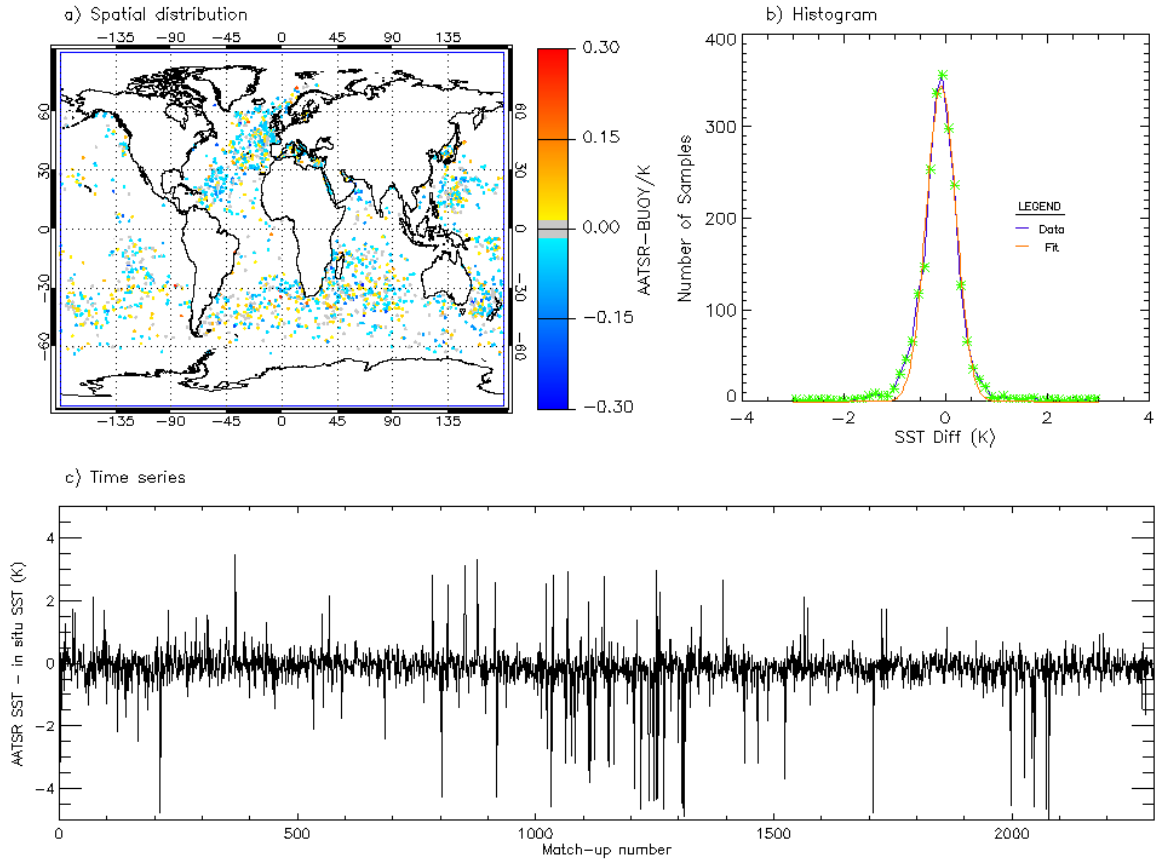

Figure 3-38: Spatial distribution, histogram and time series of Case 8 match-ups, 3-channel retrieval, $TL_3 < D\text{-}N < TU_3$, wind speed > 6 m^{-1}

The statistics for the Case 8 match-ups are given in Table 3-32. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-32: Statistics for Case 8 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	2321	-0.158	0.70	-0.100	0.35
Moored only	643	-0.176	0.55	-0.162	0.38
Ships only	7725	-0.163	1.37	-0.190	1.10
TTP* only	144	-0.168	0.28	-0.130	0.28

*TTP = TAO/TRITON/PIRATA moored buoys

3.4.11 Case 9: 3-channel retrieval, D-N < TL_3, wind speed < 6 m^{-1}

Figure 3-39 shows a) the spatial distribution of Case 9 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between ATSR-2 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

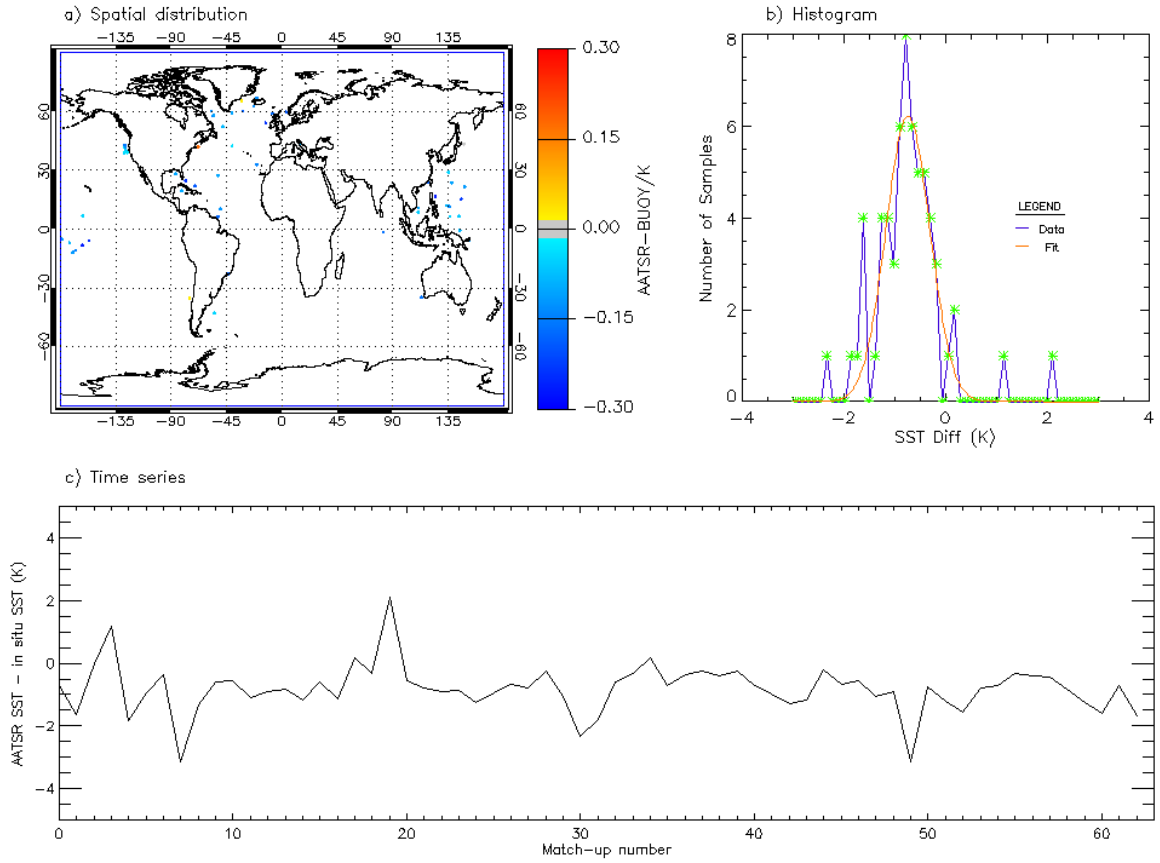

Figure 3-39: Spatial distribution, histogram and time series of Case 9 match-ups, 3-channel retrieval, D-N < TL_3, wind speed < 6 m^{-1}

The statistics for the Case 9 match-ups are given below in Table 3-33. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-33: Statistics for Case 9 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	64	+0.820	0.78	-0.789	0.57
Moored only	108	-0.326	0.52	-0.335	0.53
Ships only	235	-0.821	1.34	-0.814	1.26
TTP* only	13	-0.744	0.31	-0.690	0.26

*TTP = TAO/TRITON/PIRATA moored buoys

3.4.12 Case 10: 3-channel retrieval, D-N < TL_3, wind speed > 6 m^{-1}

Figure 3-40 shows a) the spatial distribution of Case 10 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between ATSR-2 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

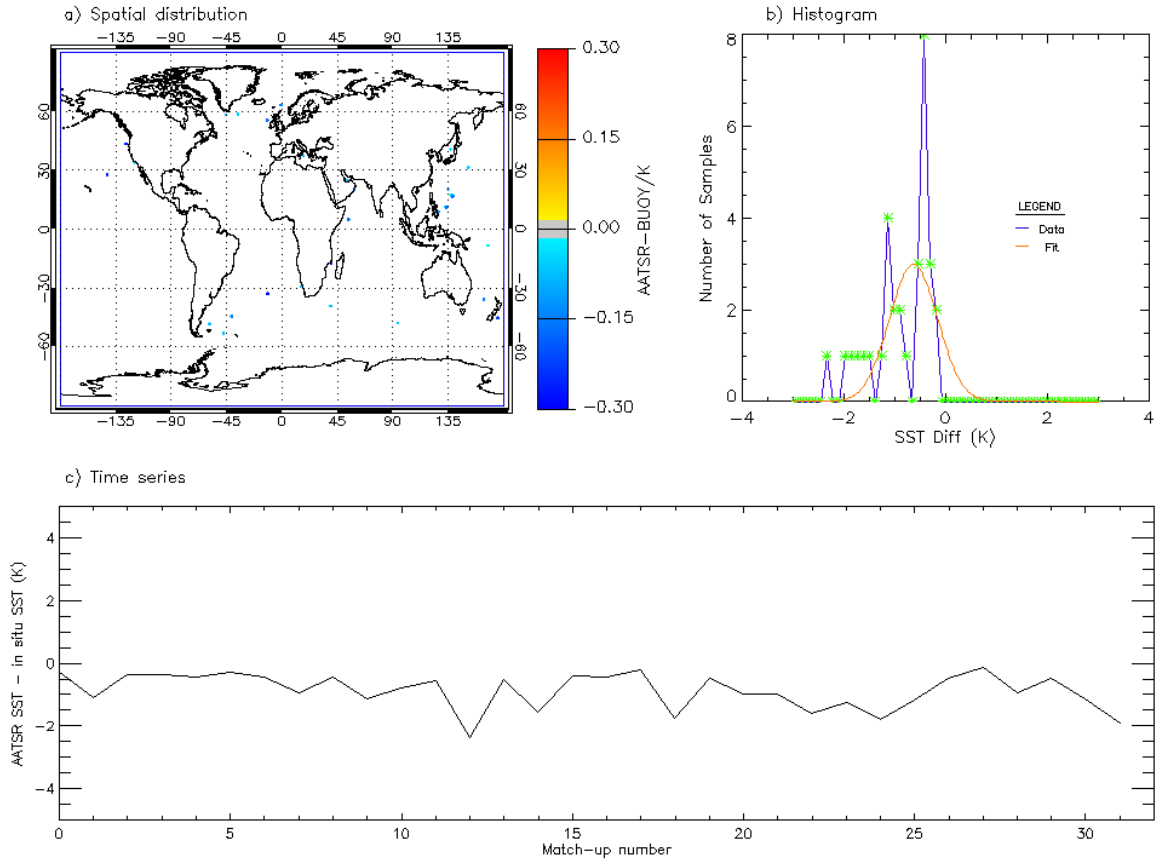

Figure 3-40: Spatial distribution, histogram and time series of Case 10 match-ups, 3-channel retrieval, D-N < TL_3, wind speed > 6 m^{-1}

The statistics for the Case 10 match-ups are given in Table 3-34. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-34: Statistics for Case 10 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	32	-0.865	0.58	-0.660	0.58
Moored only	17	-0.971	0.66	-1.009	0.68
Ships only	155	-1.222	1.39	-1.189	1.21
TTP* only	1	-0.849	-	-	-

*TTP = TAO/TRITON/PIRATA moored buoys

3.4.13 Case 11: 3-channel retrieval, D-N > TU_3, wind speed < 6 m^{-1}

Figure 3-41 shows a) the spatial distribution of Case 11 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between ATSR-2 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

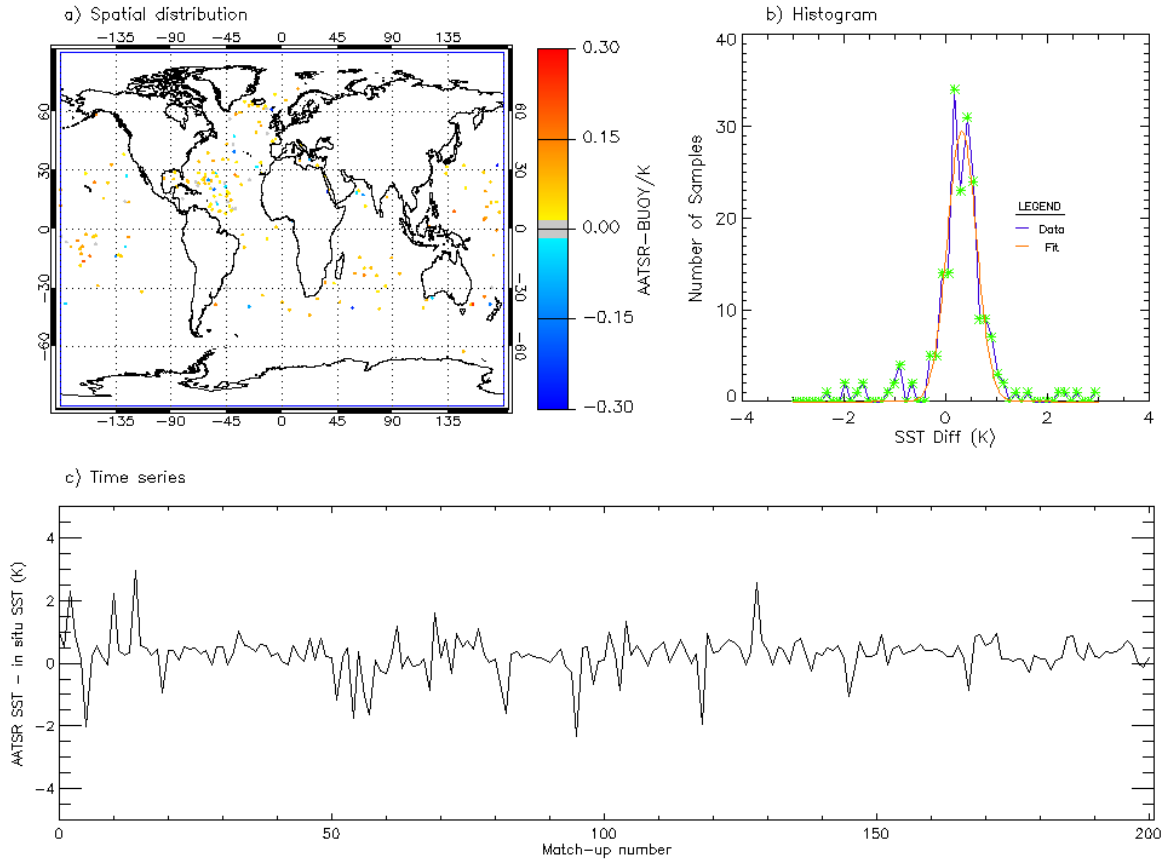

Figure 3-41: Spatial distribution, histogram and time series of Case 11 match-ups, 3-channel retrieval, D-N > TU_3, wind speed < 6 m^{-1}

The statistics for the Case 11 match-ups are given in Table 3-35. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-35: Statistics for Case 11 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	205	+0.276	0.64	+0.319	0.36
Moored only	65	+0.239	0.62	+0.335	0.40
Ships only	741	+0.335	1.40	+0.269	1.14
TTP* only	23	+0.286	0.37	+0.268	0.38

*TTP = TAO/TRITON/PIRATA moored buoys

3.4.14 Case 12: 3-channel retrieval, D-N > TU_3, wind speed > 6 m^{-1}

Figure 3-42 shows a) the spatial distribution of Case 12 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between ATSR-2 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

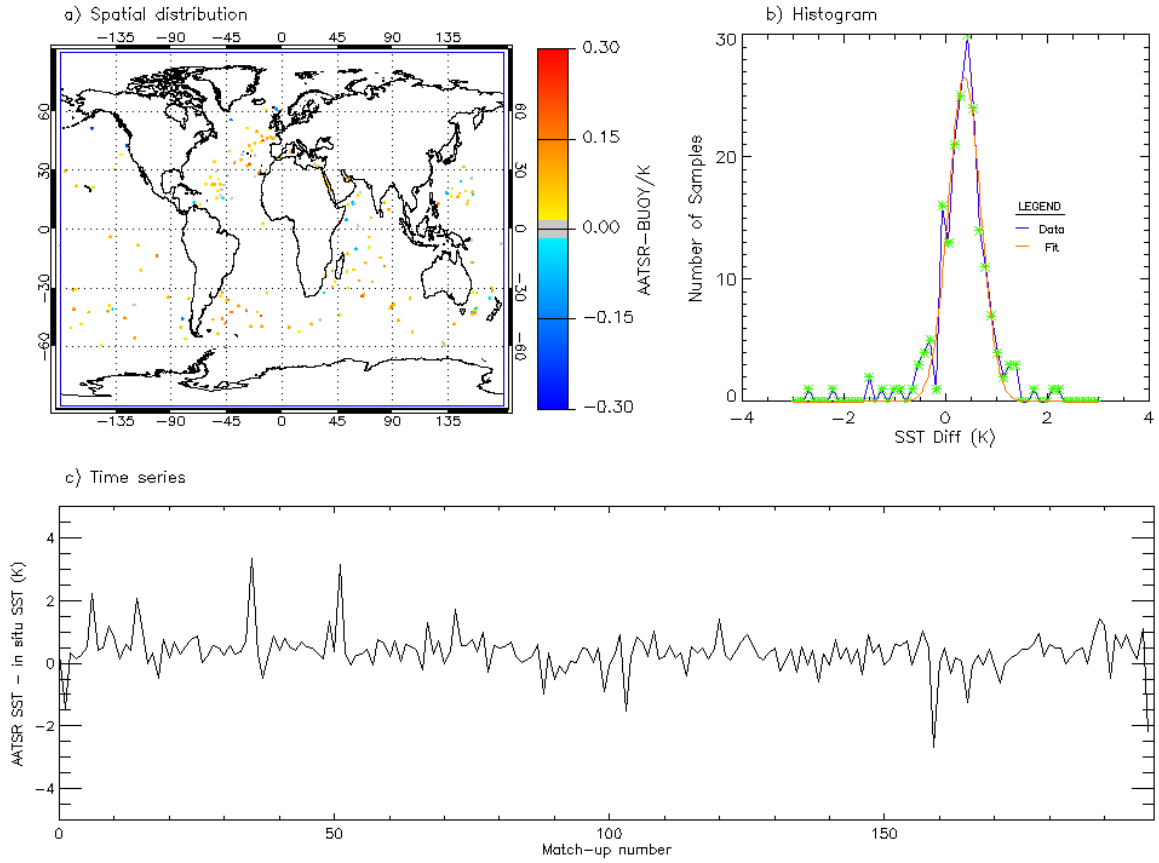

Figure 3-42: Spatial distribution, histogram and time series of Case 12 match-ups, 3-channel retrieval, D-N < TU_3, wind speed > 6 m^{-1}

The statistics for the Case 12 match-ups are given in Table 3-36. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-36: Statistics for Case 12 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	202	+0.358	0.64	+0.380	0.41
Moored only	33	+0.337	0.64	+0.479	0.39
Ships only	726	+0.260	1.46	+0.232	1.21
TTP* only	7	+0.211	0.51	+0.430	0.22

*TTP = TAO/TRITON/PIRATA moored buoys

3.4.15 Summary of the Analysis

Table 3-37 summarises the match-up statistics for all 12 cases. Additional match-up statistics are provided in tables 3-38 to 3-43, where the wind speed dependency has been removed. Inspection of tables 3-37 to 3-43 highlights the following:

- The total number of match-ups to surface drifting buoys is, in all cases, very low compared to AATSR, even though the total number of months is considerably more; the ATSR-2 MDB currently contains 45 months of match-ups, compared to 15 months for AATSR.
- As for AATSR, there is little if any wind speed dependence observed, compared to the Medspiration AATSR MDB [AD2]. Indeed, there does appear to be some wind speed dependence for day time, but the bias is lower at low speeds, implying no diurnal heating. This is somewhat surprising given that the ATSR-2 MLST is 30 minutes later than AATSR.
- If wind speed dependence is ignored, then the calculated night time biases and standard deviations are very similar to those calculated for AATSR, albeit with larger variances.
- The calculated day time 2-channel bias for data within the 3-sigma thresholds is a lot lower than observed for AATSR, and is in line with the suspected 12 µm offset in AATSR.
- The calculated biases for day time 2-channel data outside of the 3-sigma thresholds is quite different to AATSR, and might imply a failing of the D-N test. Further investigation is needed.
- The robust standard deviation is generally a lot lower than the non-robust standard deviation, indicating outliers having a strong influence. The cause of these outliers is likely to be either an issue with the SSES scheme that requires further refinement for ATSR-2, or an issue with the QC of the in situ data. Both possibilities require significant further work to better understand these outliers.

As for AATSR, the ATSR-2 SSTs are skin SSTs and so an adjustment of + 0.17 K should be added to all biases when converting tables 3-37 to 3-43 into the SSES bias values.

Table 3-37: Summary of validation statistics for all stratification cases

Data Set		Statistics				
		Number	Mean (ºC)	Sigma (ºC)	Median (ºC)	Robust Sigma (ºC)
Case 1	Drifters only	3301	-0.151	0.81	-0.100	0.43
	Moored only	2127	-0.056	0.63	-0.069	0.51
	Ships only	10987	-0.159	1.48	-0.199	1.21
	TTP* only	492	-0.125	0.34	-0.120	0.31
Case 2	Drifters only	2033	-0.129	0.76	-0.100	0.43
	Moored only	527	-0.097	0.73	-0.129	0.52
	Ships only	8649	-0.216	1.42	-0.250	1.20
	TTP* only	152	-0.133	0.30	-0.120	0.29
Case 3	Drifters only	78	-0.708	0.79	-0.540	0.74
	Moored only	55	-0.719	0.76	-0.771	0.78
	Ships only	328	-0.626	1.58	-0.629	1.42
	TTP* only	30	-0.749	0.69	-0.621	0.63
Case 4	Drifters only	46	-0.863	1.01	-0.710	0.88
	Moored only	4	-1.185	0.86	-1.439	0.97
	Ships only	217	-0.654	1.40	-0.730	1.30
	TTP* only	9	-0.418	0.37	-0.362	0.38
Case 5	Drifters only	179	-0.488	1.85	+0.051	0.89
	Moored only	106	-0.742	2.59	-0.059	1.16
	Ships only	568	-0.188	2.16	-0.039	1.80
	TTP* only	11	+0.682	0.54	+0.084	0.47
Case 6	Drifters only	89	-0.545	2.17	+0.100	0.65
	Moored only	14	-1.726	3.09	-0.100	1.27
	Ships only	476	-0.034	1.85	+0.080	1.53
	TTP* only	3	+0.516	0.58	+0.810	-
Case 7	Drifters only	2698	-0.138	0.47	-0.121	0.35
	Moored only	1829	-0.050	0.44	-0.040	0.40
	Ships only	8809	-0.152	1.34	-0.170	1.09
	TTP* only	437	-0.172	0.26	-0.160	0.25
Case 8	Drifters only	2321	-0.158	0.70	-0.100	0.35
	Moored only	643	-0.176	0.55	-0.162	0.38
	Ships only	7725	-0.163	1.37	-0.190	1.10
	TTP* only	144	-0.168	0.28	-0.130	0.28
Case 9	Drifters only	64	+0.820	0.78	-0.789	0.57
	Moored only	108	-0.326	0.52	-0.335	0.53
	Ships only	235	-0.821	1.34	-0.814	1.26
	TTP* only	13	-0.744	0.31	-0.690	0.26

Data Set		Statistics				
		Number	Mean (ºC)	Sigma (ºC)	Median (ºC)	Robust Sigma (ºC)
Case 10	Drifters only	32	-0.865	0.58	-0.660	0.58
	Moored only	17	-0.971	0.66	-1.009	0.68
	Ships only	155	-1.222	1.39	-1.189	1.21
	TTP* only	1	-0.849	-	-	-
Case 11	Drifters only	205	+0.276	0.64	+0.319	0.36
	Moored only	65	+0.239	0.62	+0.335	0.40
	Ships only	741	+0.335	1.40	+0.269	1.14
	TTP* only	23	+0.286	0.37	+0.268	0.38
Case 12	Drifters only	202	+0.358	0.64	+0.380	0.41
	Moored only	33	+0.337	0.64	+0.479	0.39
	Ships only	726	+0.260	1.46	+0.232	1.21
	TTP* only	7	+0.211	0.51	+0.430	0.22

*TTP = TAO/TRITON/PIRATA moored buoys

Table 3-38: Statistics for 2-channel retrieval, TL_2 < D-N < TU_2 (combining cases 1 and 2)

Dataset	Statistics				
	Number	Mean (°C)	Sigma (°C)	Median (°C)	Robust Sigma(°C)
Drifters only	5334	-0.146	0.79	-0.100	0.43
Moored only	2654	-0.059	0.65	-0.079	0.52
Ships only	19636	-0.183	1.45	-0.220	1.21
TTP* only	644	-0.127	0.33	-0.120	0.30

*TTP = TAO/TRITON/PIRATA moored buoys

Table 3-39: Statistics for 2-channel retrieval, D-N < TL_2 (combining cases 3 and 4)

Dataset	Statistics				
	Number	Mean (°C)	Sigma (°C)	Median (°C)	Robust Sigma(°C)
Drifters only	124	-0.736	0.82	-0.595	0.78
Moored only	59	-0.751	0.77	-0.780	0.79
Ships only	545	-0.637	1.50	-0.660	1.37
TTP* only	39	-0.618	0.55	-0.476	0.54

*TTP = TAO/TRITON/PIRATA moored buoys

Table 3-40: Statistics for 2-channel retrieval, D-N > TU_2 (combining cases 5 and 6)

Dataset	Statistics				
	Number	Mean (°C)	Sigma (°C)	Median (°C)	Robust Sigma(°C)
Drifters only	268	-0.542	2.03	+0.061	0.82
Moored only	120	-0.789	2.57	+0.058	1.14
Ships only	1044	-0.102	2.02	+0.011	1.66
TTP* only	14	+0.646	0.53	+0.825	0.48

*TTP = TAO/TRITON/PIRATA moored buoys

Table 3-41: Statistics for 3-channel retrieval, TL_3 < D-N < TU_3 (combining cases 7 and 8)

Dataset	Statistics				
	Number	Mean (°C)	Sigma (°C)	Median (°C)	Robust Sigma(°C)
Drifters only	5019	-0.140	0.59	-0.111	0.35
Moored only	2472	-0.089	0.48	-0.072	0.40
Ships only	16534	-0.159	1.36	-0.180	1.09
TTP* only	581	-0.171	0.27	-0.149	0.26

*TTP = TAO/TRITON/PIRATA moored buoys

Table 3-42: Statistics for 3-channel retrieval, D-N < TL_3 (combining cases 9 and 10)

Dataset	Statistics				
	Number	Mean (°C)	Sigma (°C)	Median (°C)	Robust Sigma(°C)
Drifters only	96	-0.835	0.72	-0.780	0.57
Moored only	125	-0.429	0.60	-0.375	0.61
Ships only	390	-0.979	1.43	-0.888	1.27
TTP* only	14	-0.752	0.30	-0.714	0.27

*TTP = TAO/TRITON/PIRATA moored buoys

Table 3-43: Statistics for 3-channel retrieval, D-N > TU_3 (combining cases 11 and 12)

Dataset	Statistics				
	Number	Mean (°C)	Sigma (°C)	Median (°C)	Robust Sigma(°C)
Drifters only	407	+0.309	0.66	+0.341	0.39
Moored only	98	+0.271	0.62	+0.352	0.41
Ships only	1467	+0.297	1.43	+0.250	1.17
TTP* only	30	+0.268	0.40	+0.301	0.39

*TTP = TAO/TRITON/PIRATA moored buoys

3.5 ATSR-1

This section summarises the calculation of the D-N thresholds for ATSR-1, analysis of the ATSR-1 MDB and determination of the ATSR-1 SSES.

3.5.1 Calculation of D-N thresholds

The ATSR-1 D-N thresholds are derived using the same method developed for AATSR, from analysis of relatively aerosol free months October 1991 to March 1992, and October 1993 to March 1994, for the Caribbean and the Bay of Biscay. Two different years are used owing to the failure of the 3.7 micron channel. The histograms of the D-N differences are shown in Figure 3-43, and a summary of the thresholds is given in Table 3-44.

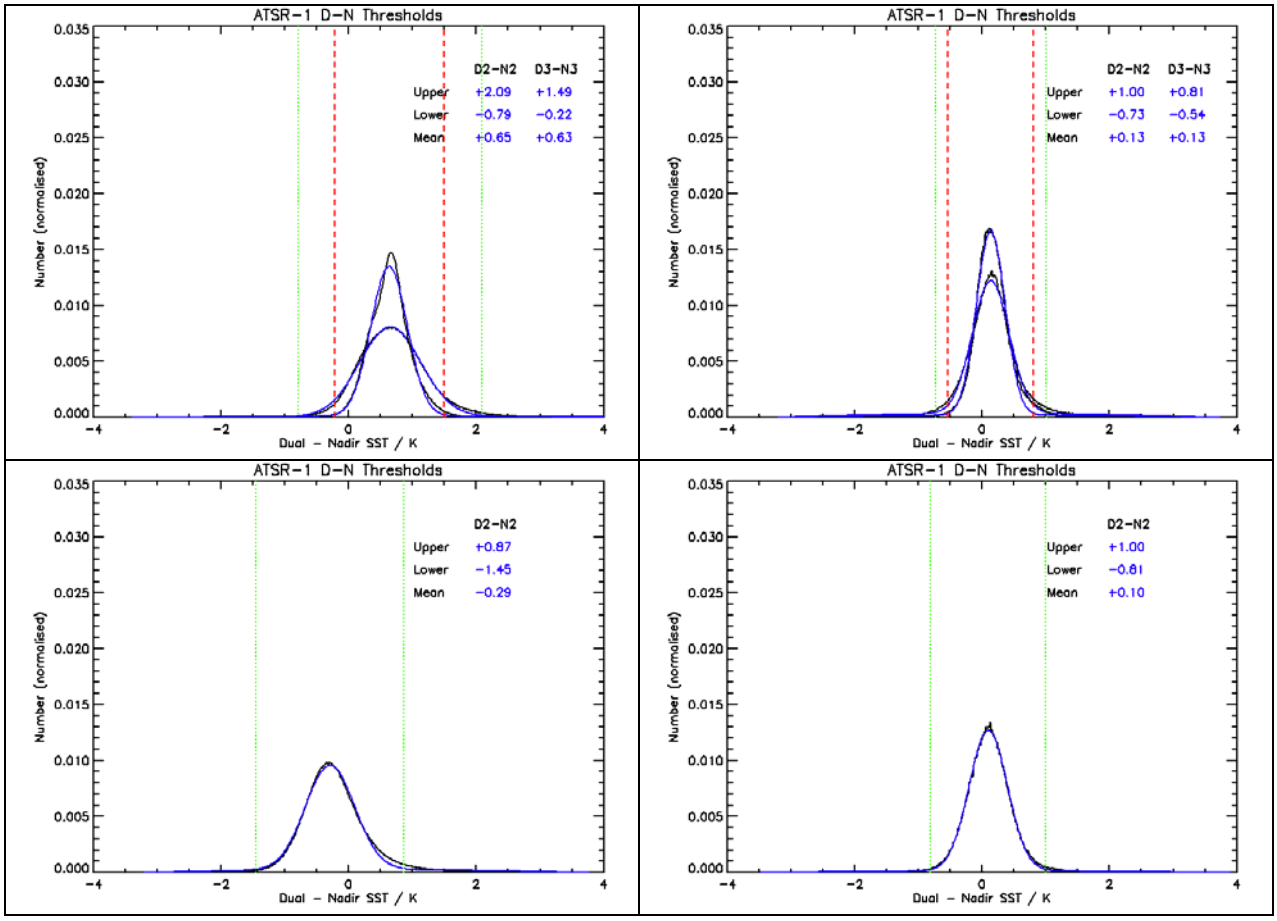

Figure 3-43: Histogram of D-N differences for D2-N2 and D3-N3 SST retrievals at full resolution for relatively aerosol-clear months of October 1991 to March 1992 for the Caribbean (upper left) and the Bay of Biscay (upper right), and for October 1993 to March 1994 for the Caribbean (lower left) and the Bay of Biscay (lower right). The 3-sigma limits for D2-N2 are indicated by the green dotted lines, and the 3-sigma limits for D3-N3 are indicated by the red dashed lines. There are no D3-N3 plots for October 1993 to March 1994 owing to the failure of the 3.7 µm channel.

	D2-N2		D3-N3	
Region	**Upper**	**Lower**	**Upper**	**Lower**
Caribbean 10/91 to 03/92	+2.09	-0.79	+1.79	-0.42
Caribbean 10/93 to 03/94	+0.87	-1.45	-	-
Biscay 10/91 to 03/92	+1.00	-0.73	+0.81	-0.54
Biscay 10/93 to 03/94	+1.00	-0.81	-	-

Table 3-44: Summary of D-N thresholds

For the global threshold, a mean value is taken and a standard error is applied. The final ATSR-1 D-N thresholds are:

- TU_2 = + 1.24 ± 0.57 K
- TL_2 = - 0.95 ± 0.34 K
- TU_3 = + 1.15 ± 0.69 K
- TL_3 = - 0.38 ± 0.08 K

The histograms and calculated thresholds are quite different to the later instruments. In particular the presence of stratospheric aerosols from the eruption of Mount Pinatubo causes a notable shift in the Caribbean thresholds for 1991 to 1992. Also, it is noted that the relative difference between the D2-N2 and D3-N3 thresholds is very small, compared to that observed for the later instruments.

3.5.2 Analysis of MDB

A basic analysis of the ATSR-1 MDB was carried out using the method derived for AATSR and the ATSR-1 D-N thresholds. As for AATSR, a ± 3 sigma filter is applied before calculating the mean bias and standard deviation to remove any remaining outliers that would otherwise overly affect the statistics. Both robust and non-robust statistics are reported.

It is noted that owing to the failure of the 3.7 µm channel, 2-channel SSES can be produced for night time data, which will have considerably less influence from diurnal heating, thus providing improved 2-channel SSES. Day time 2-channel SSES are still calculated and are reported here for completeness. The night time 2-channel SSES will be used in the ATSR-1 L2P data.

3.5.3 Case 1: 2-channel retrieval day time, $TL_2 < D\text{-}N < TU_2$, wind speed < 6 m^{-1}

Figure 3-44 shows (a) the spatial distribution of Case 1 match-ups, (b) the histogram of the match-ups (together with a fitted Gaussian), and (c) a time series of the differences between ATSR-1 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

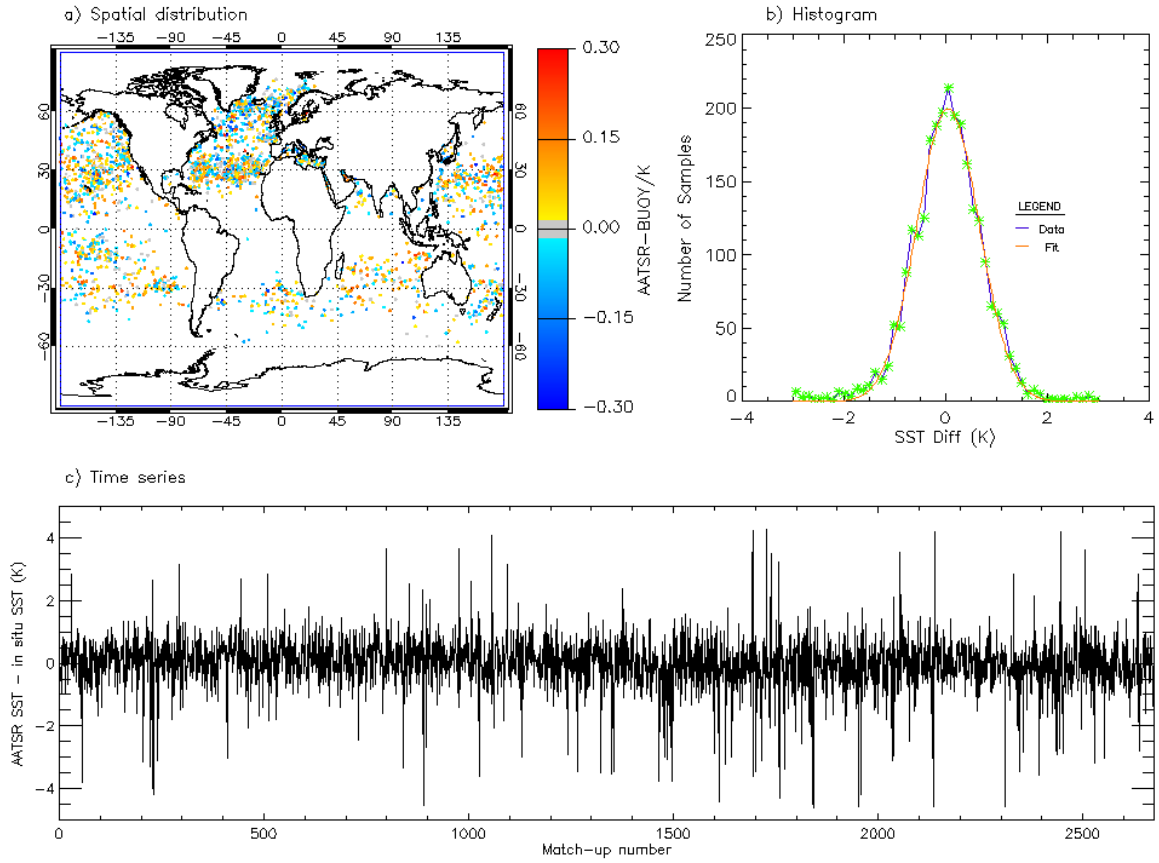

Figure 3-44: Spatial distribution, histogram and time series of Case 1 match-ups, 2-channel retrieval, $TL_2 < D\text{-}N < TU_2$, wind speed < 6 m^{-1}

The statistics for the Case 1 match-ups are given in Table 3-45. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-45: Statistics for Case 1 match-ups

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	2734	-0.007	0.88	+0.030	0.68
Moored only	2787	-0.012	0.84	+0.018	0.74
Ships only	20197	-0.065	1.58	-0.048	1.39
TTP* only	1250	+0.034	0.54	+0.018	0.53

*TTP = TAO/TRITON/PIRATA moored buoys

3.5.4 Case 2: 2-channel retrieval day time, $TL_2 < D\text{-}N < TU_2$, wind speed > 6 m^{-1}

Figure 3-46 shows a) the spatial distribution of Case 2 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between ATSR-1 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

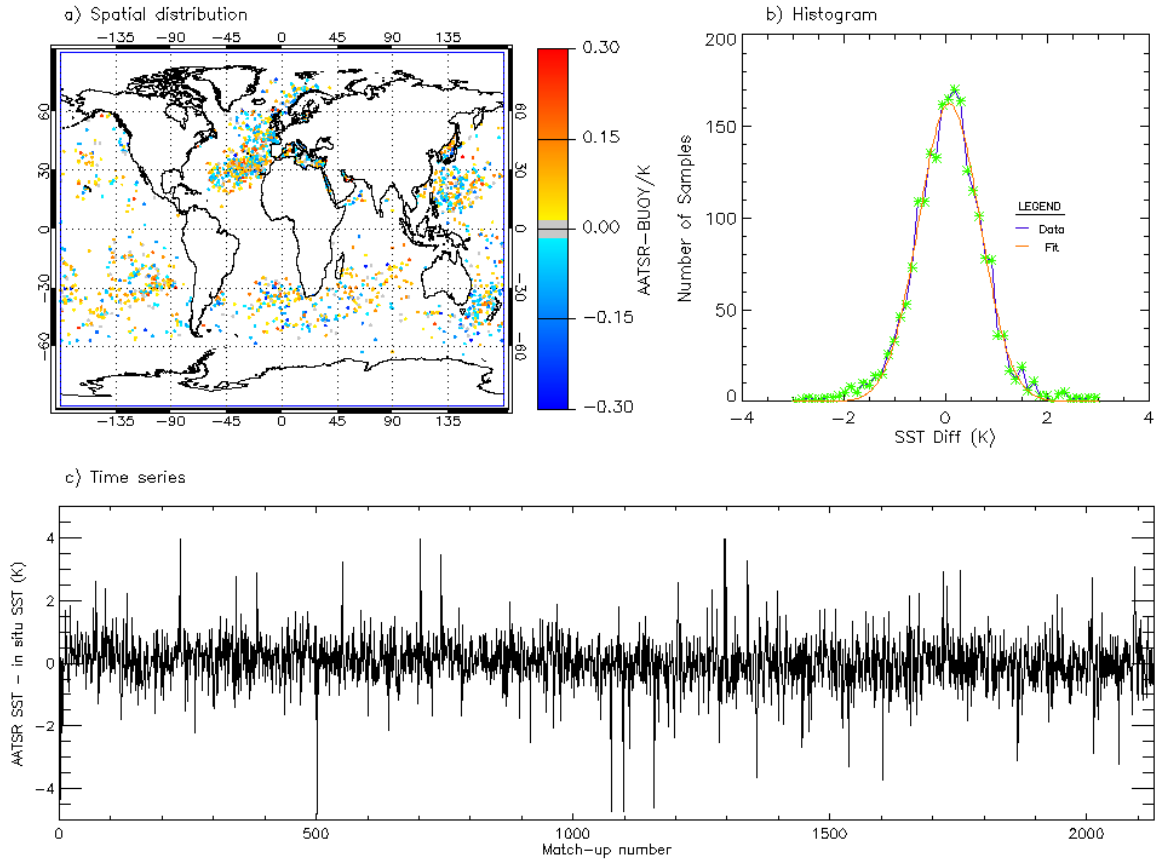

Figure 3-45: Spatial distribution, histogram and time series of Case 2 match-ups, 2-channel retrieval, $TL_2 < D\text{-}N < TU_2$, wind speed > 6 m^{-1}

The statistics for the Case 2 match-ups are given below in Table 3-46. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-46: Statistics for Case 2 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	2156	+0.054	0.79	+0.070	0.67
Moored only	765	-0.102	0.97	-0.055	0.74
Ships only	16193	-0.098	1.51	-0.090	1.34
TTP* only	300	-0.017	0.56	-0.005	0.56

*TTP = TAO/TRITON/PIRATA moored buoys

3.5.5 Case 3: 2-channel retrieval day time, D-N < TL_2, wind speed < 6 m^{-1}

Figure 3-46 shows a) the spatial distribution of Case 3 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between ATSR-1 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

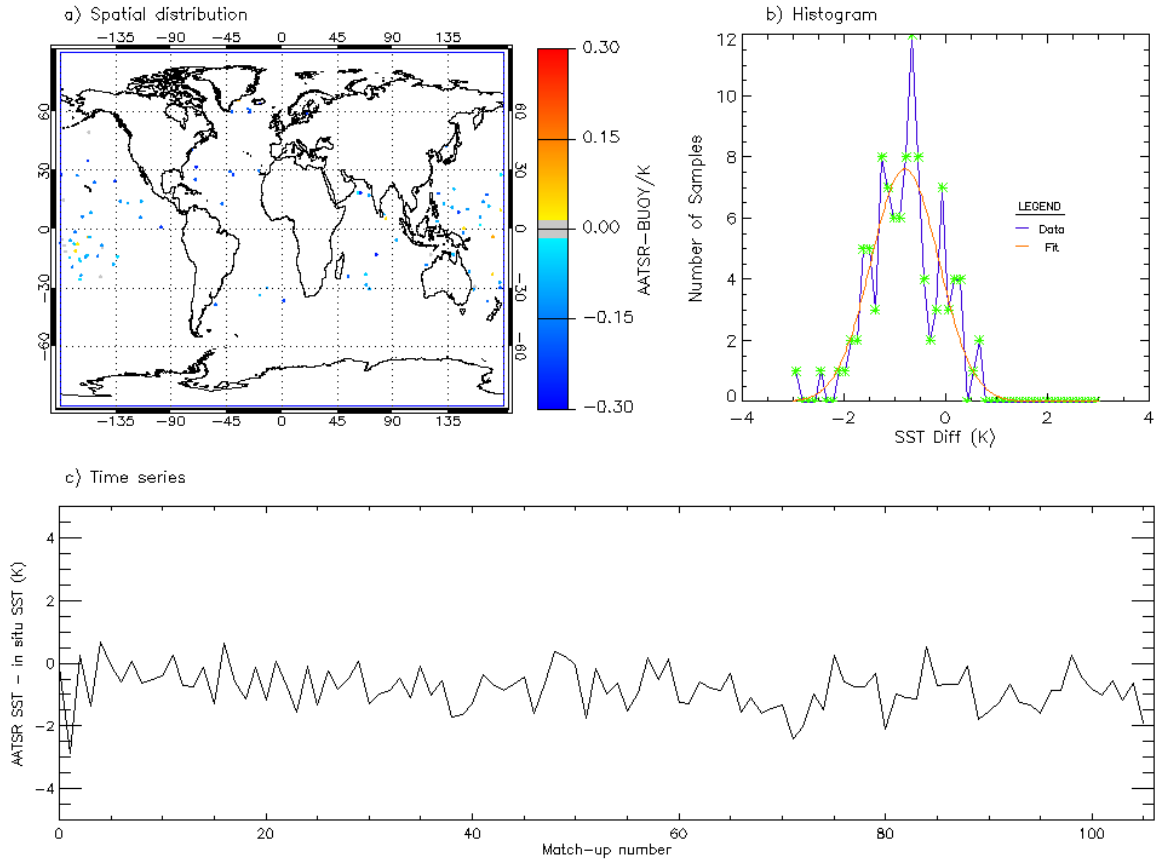

Figure 3-46: Spatial distribution, histogram and time series of Case 3 match-ups, 2-channel retrieval, D-N < TL_2, wind speed < 6 m^{-1}

The statistics for the Case 3 match-ups are given below in Table 3-47. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-47: Statistics for Case 3 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	108	-0.786	0.67	-0.755	0.67
Moored only	81	-1.191	0.85	-1.130	0.83
Ships only	1065	-0.595	1.52	-0.581	1.40
TTP* only	319	-0.507	0.53	-0.480	0.52

*TTP = TAO/TRITON/PIRATA moored buoys

3.5.6 Case 4: 2-channel retrieval day time, D-N < TL_2, wind speed > 6 m^{-1}

Figure 3-47 below shows a) the spatial distribution of Case 4 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between ATSR-1 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

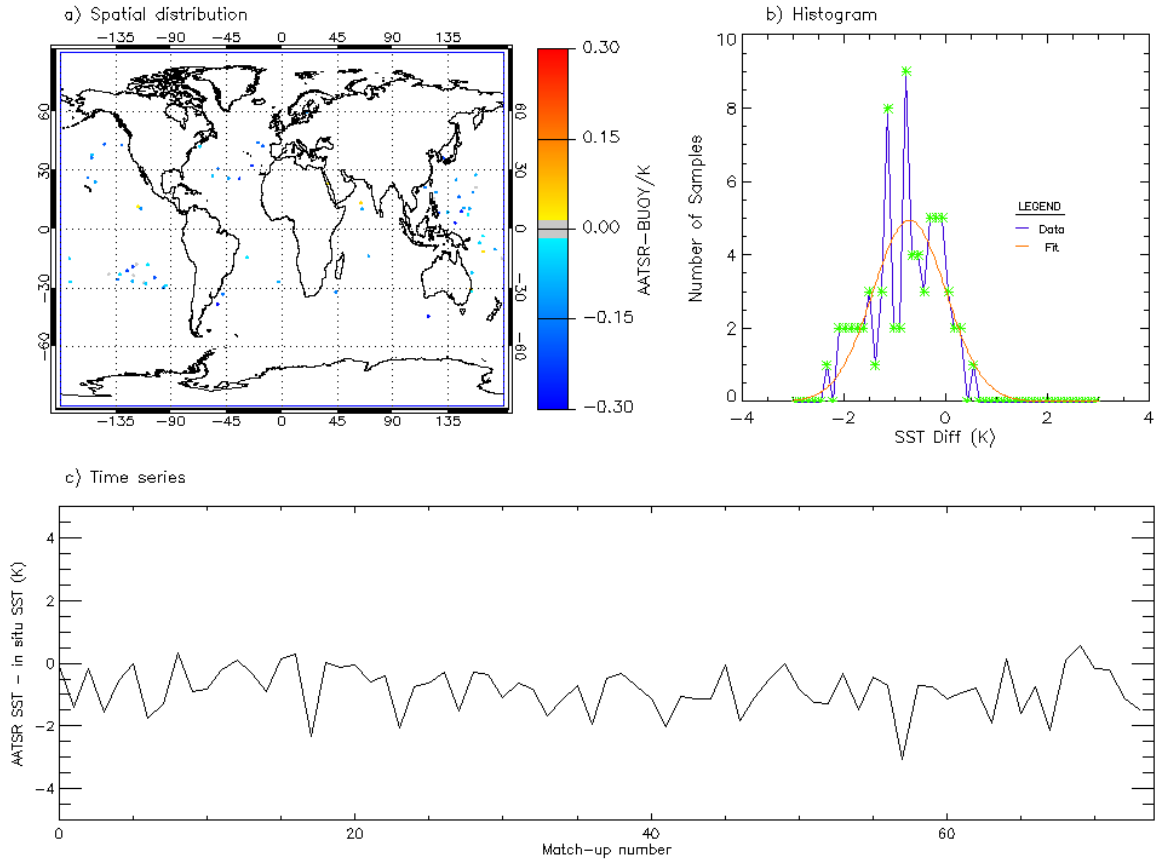

Figure 3-47: Spatial distribution, histogram and time series of Case 4 match-ups, 2-channel retrieval, D-N < TL_2, wind speed > 6 m^{-1}

The statistics for the Case 4 match-ups are given in Table 3-48. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-48: Statistics for Case 4 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	75	-0.818	0.72	-0.755	0.72
Moored only	13	-1.328	1.12	-1.292	1.11
Ships only	649	-0.781	1.44	-0.761	1.39
TTP* only	68	-0.529	0.60	-0.429	0.53

*TTP = TAO/TRITON/PIRATA moored buoys

3.5.7 Case 5: 2-channel retrieval day time, D-N > TU_2, wind speed < 6 m^{-1}

Figure 3-48 shows a) the spatial distribution of Case 5 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between ATSR-1 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

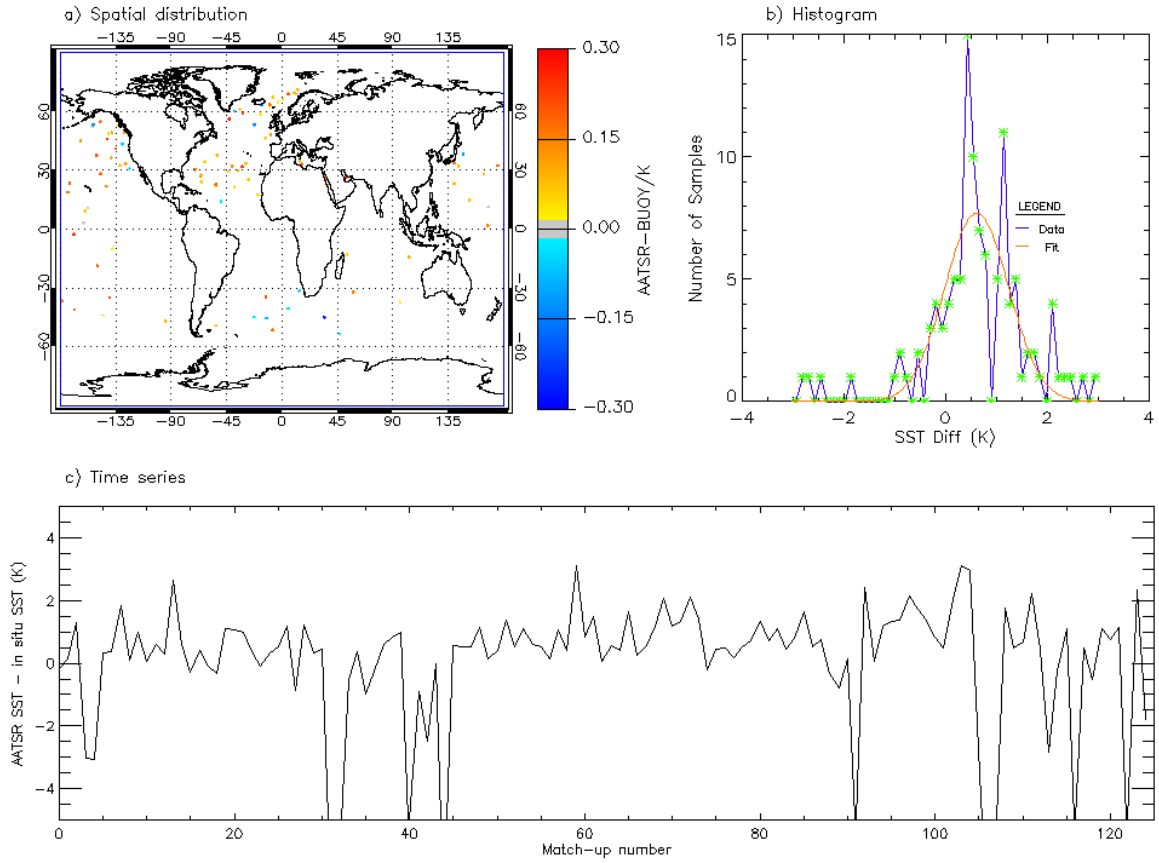

Figure 3-48: Spatial distribution, histogram and time series of Case 5 match-ups, 2-channel retrieval, D-N > TU_2, wind speed < 6 m^{-1}

The statistics for the Case 5 match-ups are given in Table 3-49. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-49: Statistics for Case 5 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	128	+0.094	2.11	+0.521	0.98
Moored only	120	+0.782	1.32	+0.778	1.05
Ships only	1371	+0.364	1.88	+0.452	1.63
TTP* only	25	+0.510	0.83	+0.331	0.81

*TTP = TAO/TRITON/PIRATA moored buoys

3.5.8 Case 6: 2-channel retrieval day time, D-N > TU_2, wind speed > 6 m^{-1}

Figure 3-49 shows a) the spatial distribution of Case 6 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between ATSR-1 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

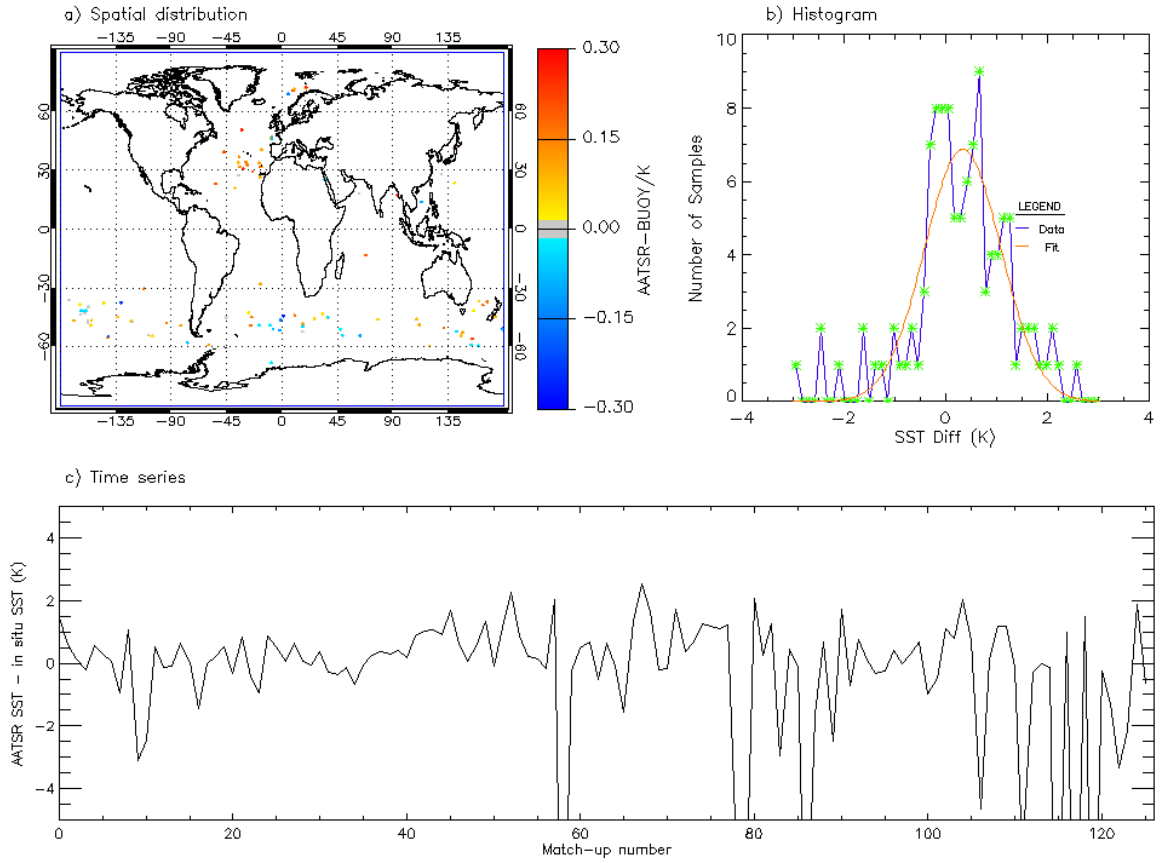

Figure 3-49: Spatial distribution, histogram and time series of Case 6 match-ups, 2-channel retrieval, D-N > TU_2, wind speed > 6 m^{-1}

The statistics for the Case 6 match-ups are given in Table 3-50. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-50: Statistics for Case 6 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	130	-0.457	2.83	+0.190	0.99
Moored only	35	+0.245	2.60	+0.635	1.28
Ships only	1312	+0.228	1.88	+0.280	1.64
TTP* only	13	+0.557	0.80	+0.410	0.79

*TTP = TAO/TRITON/PIRATA moored buoys

3.5.9 Case 1: 2-channel retrieval night time, $TL_2 < D\text{-}N < TU_2$, wind speed < 6 m^{-1}

Figure 3-50 shows (a) the spatial distribution of Case 1 match-ups, (b) the histogram of the match-ups (together with a fitted Gaussian), and (c) a time series of the differences between ATSR-1 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

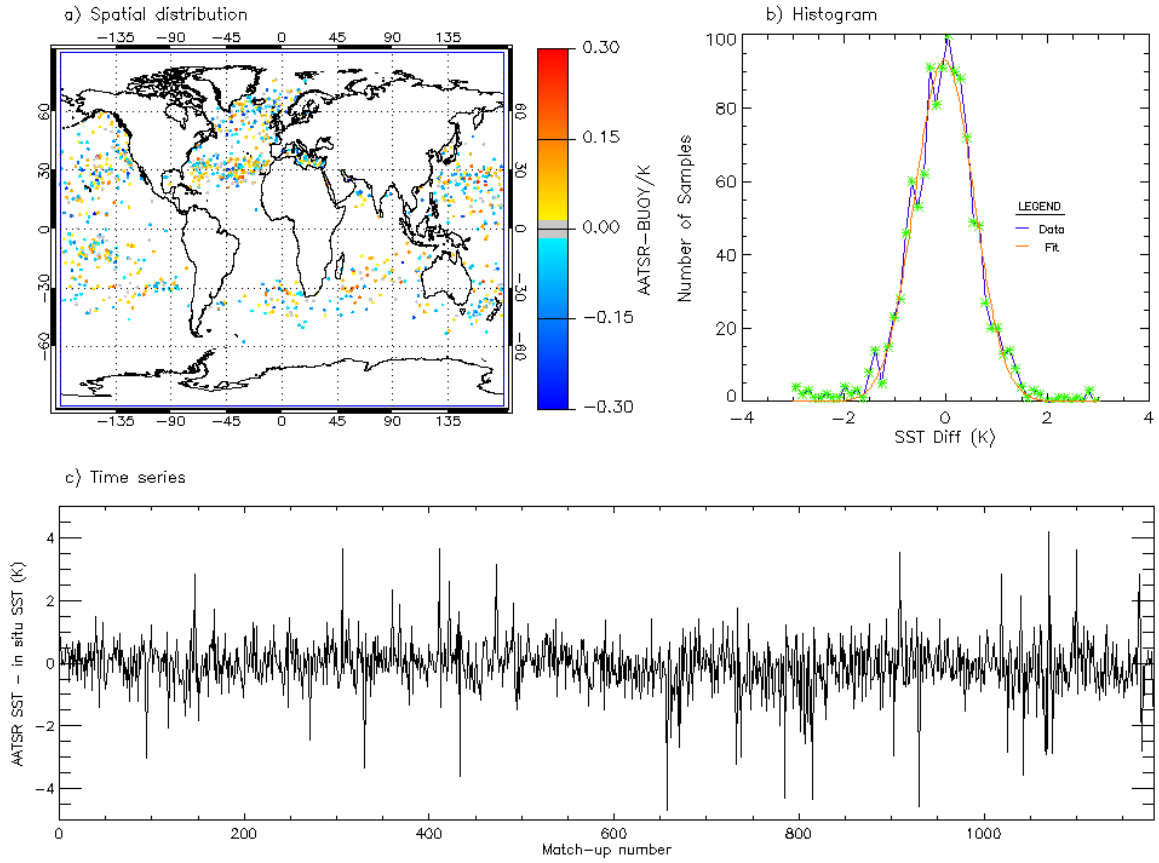

Figure 3-50: Spatial distribution, histogram and time series of Case 1 match-ups, 2-channel retrieval, $TL_2 < D\text{-}N < TU_2$, wind speed < 6 m^{-1}

The statistics for the Case 1 match-ups are given in Table 3-51. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-51: Statistics for Case 1 match-ups

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	1211	-0.069	0.83	-0.029	0.65
Moored only	1169	-0.093	0.87	-0.051	0.73
Ships only	7786	-0.137	1.59	-0.100	1.38
TTP* only	740	-0.062	0.52	-0.082	0.52

*TTP = TAO/TRITON/PIRATA moored buoys

3.5.10 Case 2: 2-channel retrieval night time, $TL_2 < D\text{-}N < TU_2$, wind speed > 6 m^{-1}

Figure 3-51 shows a) the spatial distribution of Case 2 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between ATSR-1 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

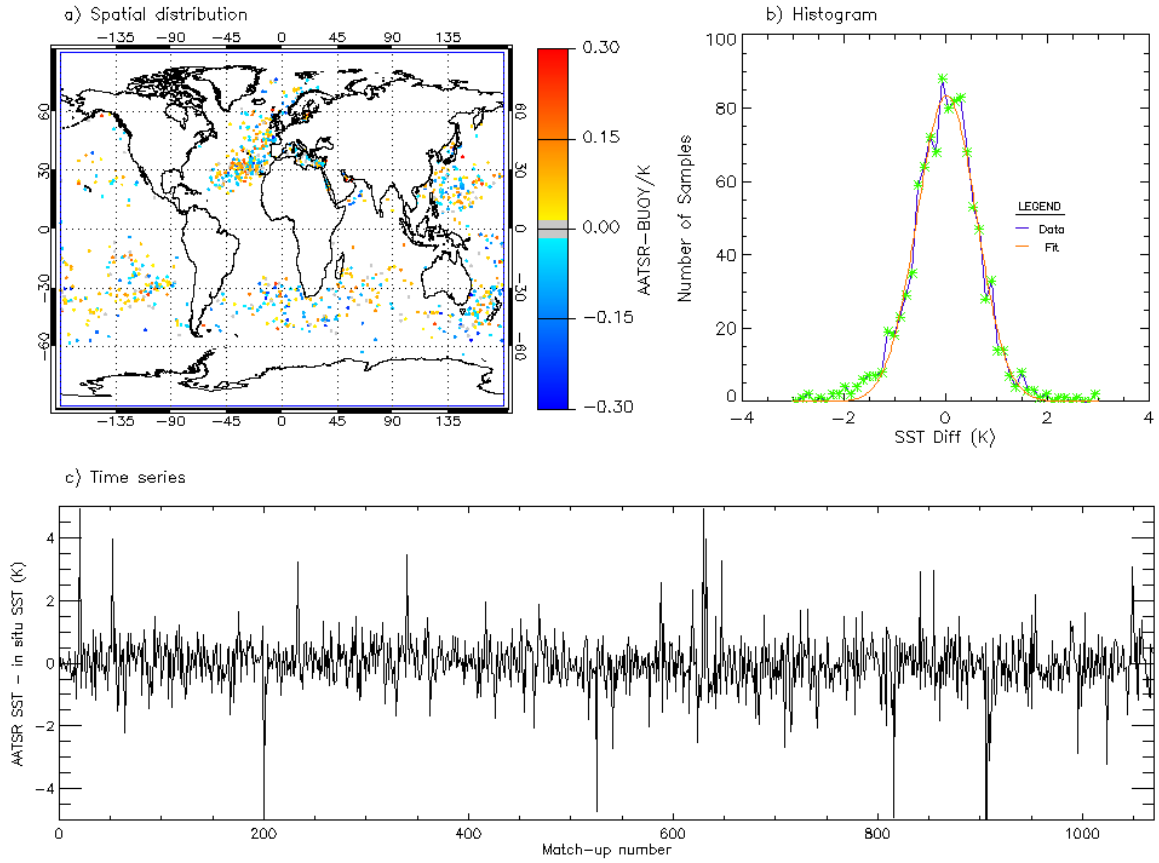

Figure 3-51: Spatial distribution, histogram and time series of Case 2 match-ups, 2-channel retrieval, $TL_2 < D\text{-}N < TU_2$, wind speed > 6 m^{-1}

The statistics for the Case 2 match-ups are given below in Table 3-52. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-52: Statistics for Case 2 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	1084	-0.007	0.84	+0.001	0.65
Moored only	376	-0.183	0.90	-0.129	0.70
Ships only	6494	-0.126	1.45	-0.090	1.32
TTP* only	180	-0.106	0.61	-0.100	0.60

*TTP = TAO/TRITON/PIRATA moored buoys

3.5.11 Case 3: 2-channel retrieval night time, D-N < TL_2, wind speed < 6 m^{-1}

Figure 3-52 shows a) the spatial distribution of Case 3 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between ATSR-1 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

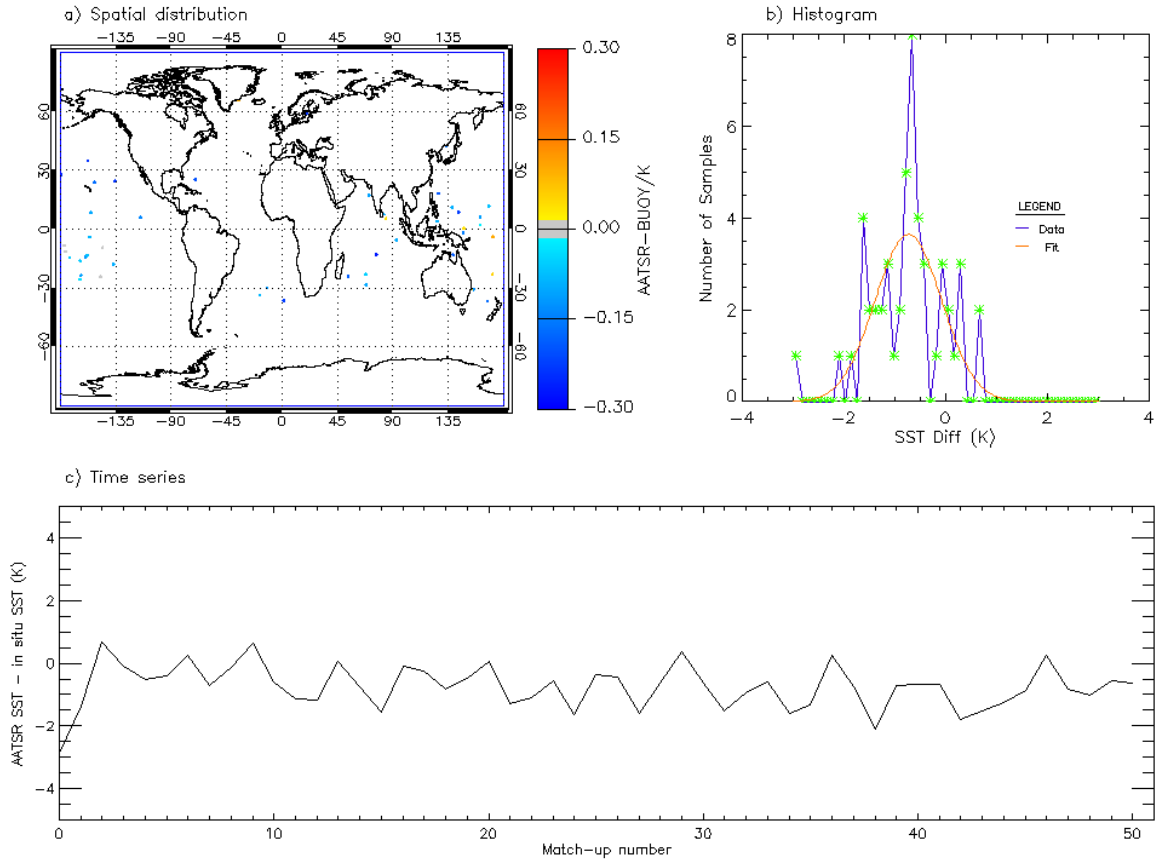

Figure 3-52: Spatial distribution, histogram and time series of Case 3 match-ups, 2-channel retrieval, D-N < TL_2, wind speed < 6 m^{-1}

The statistics for the Case 3 match-ups are given below in Table 3-53. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-53: Statistics for Case 3 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	52	-0.746	0.71	-0.681	0.70
Moored only	30	-1.203	0.86	-1.232	0.78
Ships only	422	-0.573	1.54	-0.595	1.49
TTP* only	189	-0.576	0.52	-0.560	0.52

*TTP = TAO/TRITON/PIRATA moored buoys

3.5.12 Case 4: 2-channel retrieval night time, D-N < TL_2, wind speed > 6 m^{-1}

Figure 3-53 below shows a) the spatial distribution of Case 4 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between ATSR-1 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

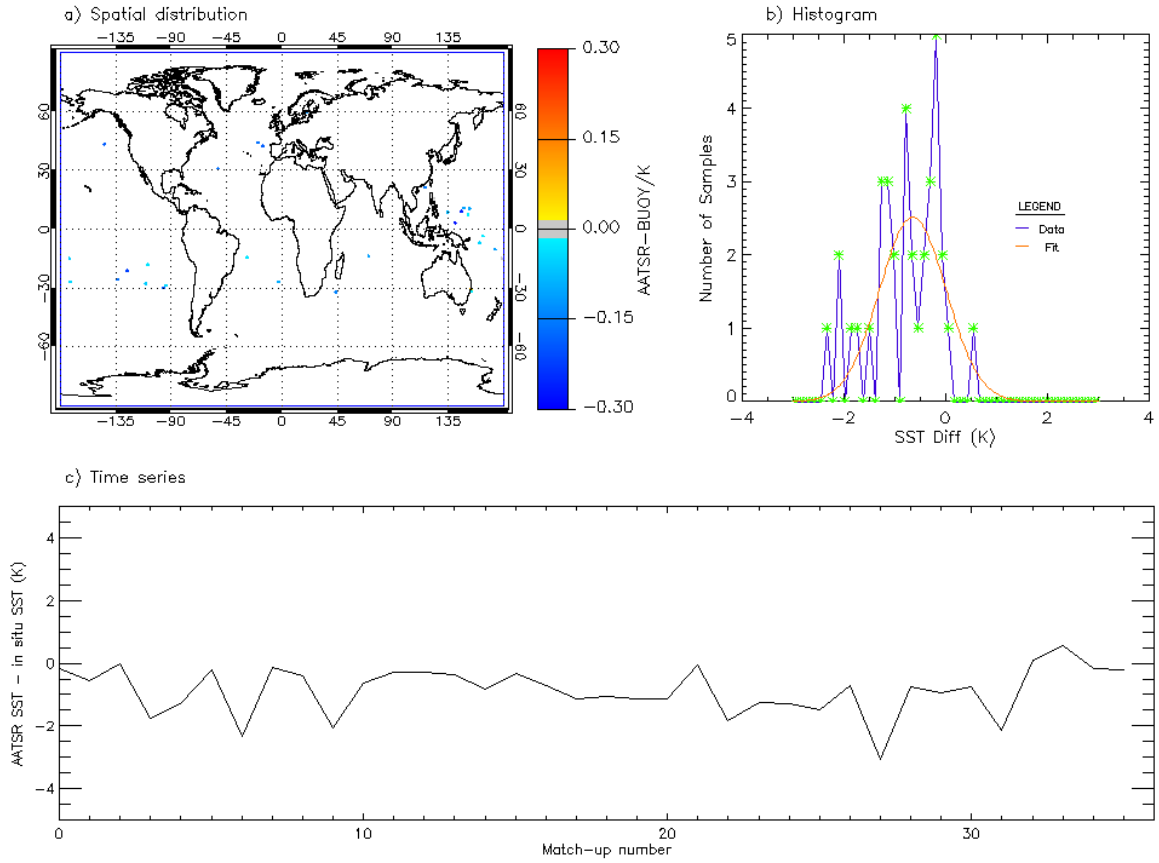

Figure 3-53: Spatial distribution, histogram and time series of Case 4 match-ups, 2-channel retrieval, D-N < TL_2, wind speed > 6 m^{-1}

The statistics for the Case 4 match-ups are given in Table 3-54. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-54: Statistics for Case 4 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	36	-0.857	0.78	-0.735	0.77
Moored only	7	-1.863	0.97	-1.708	1.02
Ships only	284	-0.740	1.45	-0.750	1.37
TTP* only	38	-0.670	0.59	-0.558	0.56

*TTP = TAO/TRITON/PIRATA moored buoys

3.5.13 Case 5: 2-channel retrieval night time, D-N > TU_2, wind speed < 6 m^{-1}

Figure 3-54 shows a) the spatial distribution of Case 5 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between ATSR-1 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

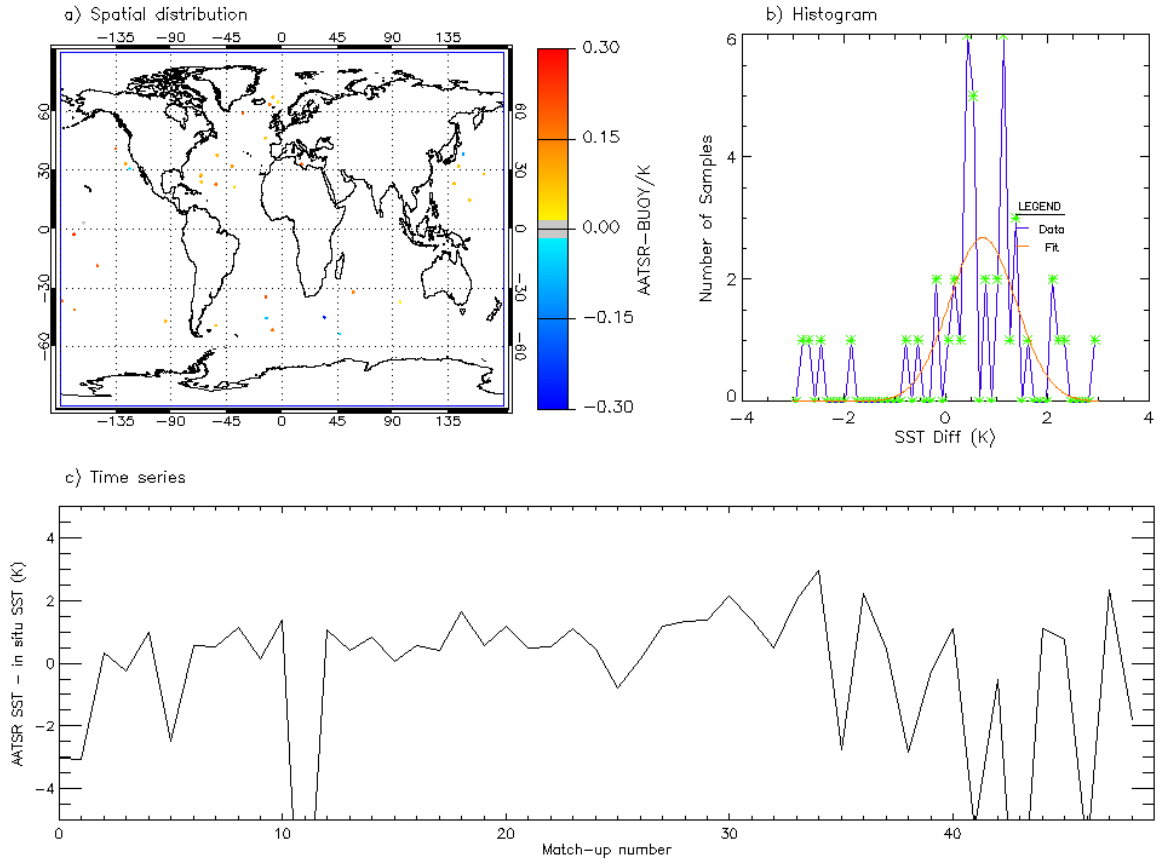

Figure 3-54: Spatial distribution, histogram and time series of Case 5 match-ups, 2-channel retrieval, D-N > TU_2, wind speed < 6 m^{-1}

The statistics for the Case 5 match-ups are given in Table 3-55. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-55: Statistics for Case 5 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	50	-0.308	2.84	+0.522	1.30
Moored only	48	+0.970	1.01	+0.988	0.84
Ships only	398	+0.475	1.87	+0.531	1.60
TTP* only	8	+1.025	1.04	+0.858	1.14

*TTP = TAO/TRITON/PIRATA moored buoys

3.5.14 Case 6: 2-channel retrieval night time, D-N > TU_2, wind speed > 6 m^{-1}

Figure 3-55 shows a) the spatial distribution of Case 6 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between ATSR-1 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

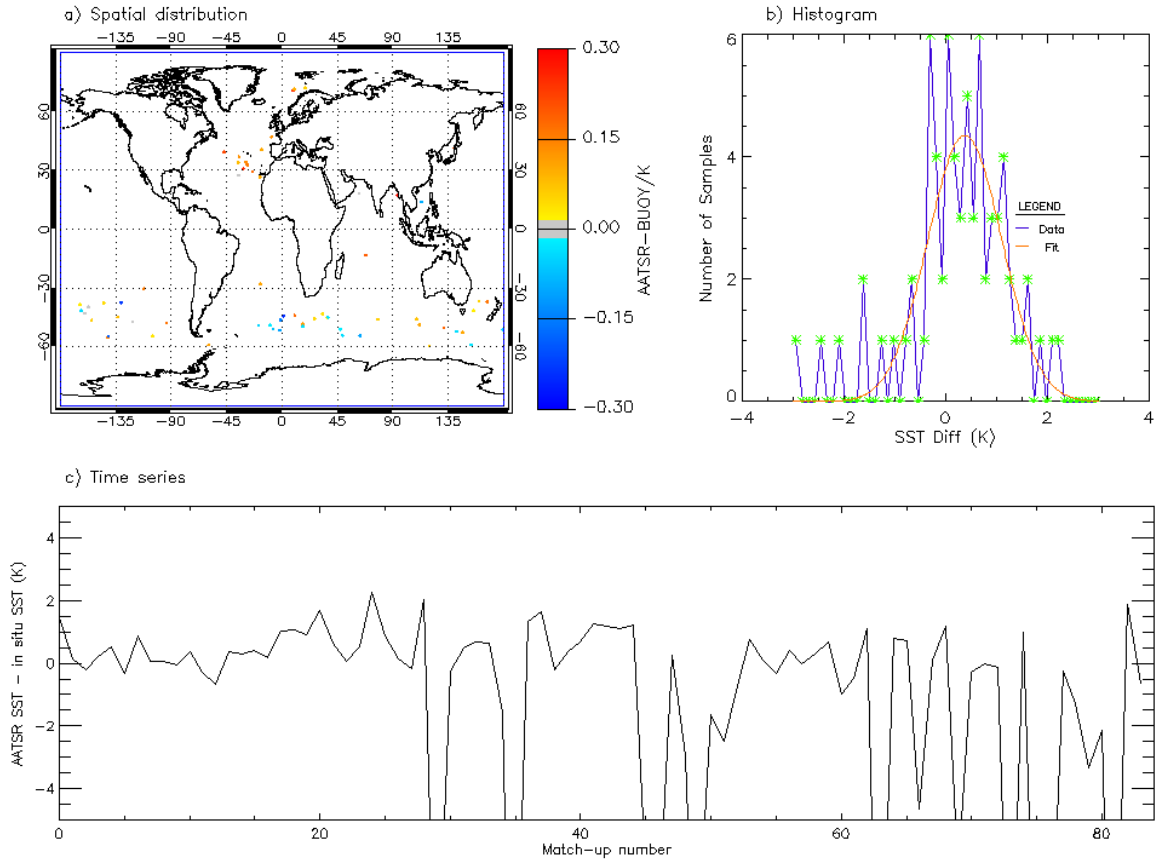

Figure 3-55: Spatial distribution, histogram and time series of Case 6 match-ups, 2-channel retrieval, D-N > TU_2, wind speed > 6 m^{-1}

The statistics for the Case 6 match-ups are given in Table 3-56. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-56: Statistics for Case 6 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	85	-1.361	4.18	+0.120	1.10
Moored only	9	-0.970	4.52	+0.332	0.86
Ships only	401	+0.432	1.95	+0.510	1.77
TTP* only	3	+0.473	1.42	+0.018	1.73

*TTP = TAO/TRITON/PIRATA moored buoys

3.5.15 Case 7: 3-channel retrieval, TL_3 < D-N < TU_3, wind speed < 6 m^{-1}

Figure 3-56 shows a) the spatial distribution of Case 7 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between ATSR-1 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

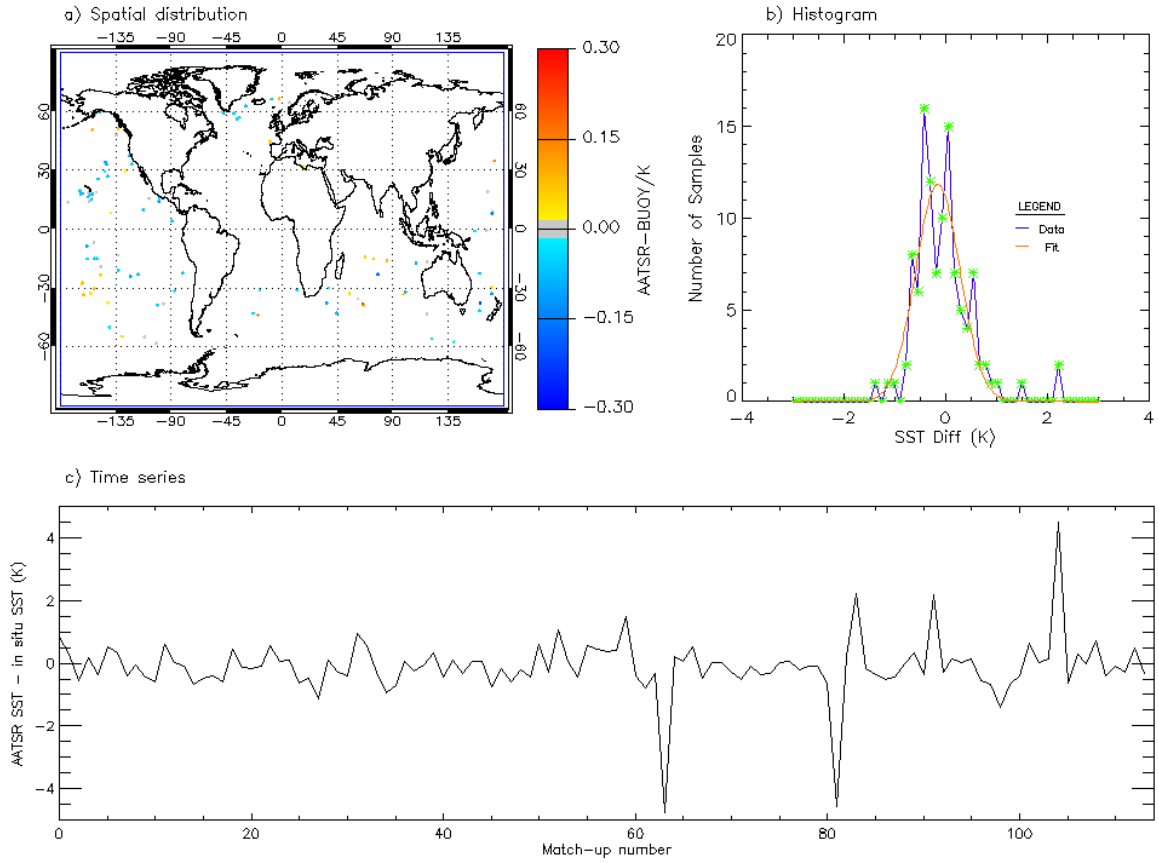

Figure 3-56: Spatial distribution, histogram and time series of Case 7 match-ups, 3-channel retrieval, TL_3 < D-N < TU_3, wind speed < 6 m^{-1}

The statistics for the Case 7 match-ups are given in Table 3-57. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-57: Statistics for Case 7 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	115	-0.098	0.93	-0.111	0.48
Moored only	171	-0.060	0.50	-0.056	0.46
Ships only	1524	-0.172	1.42	-0.150	1.25
TTP* only	42	-0.205	0.38	-0.165	0.35

*TTP = TAO/TRITON/PIRATA moored buoys

3.5.16 Case 8: 3-channel retrieval, TL_3 < D-N < TU_3, wind speed > 6 m^{-1}

Figure 3-57 shows a) the spatial distribution of Case 8 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between ATSR-1 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

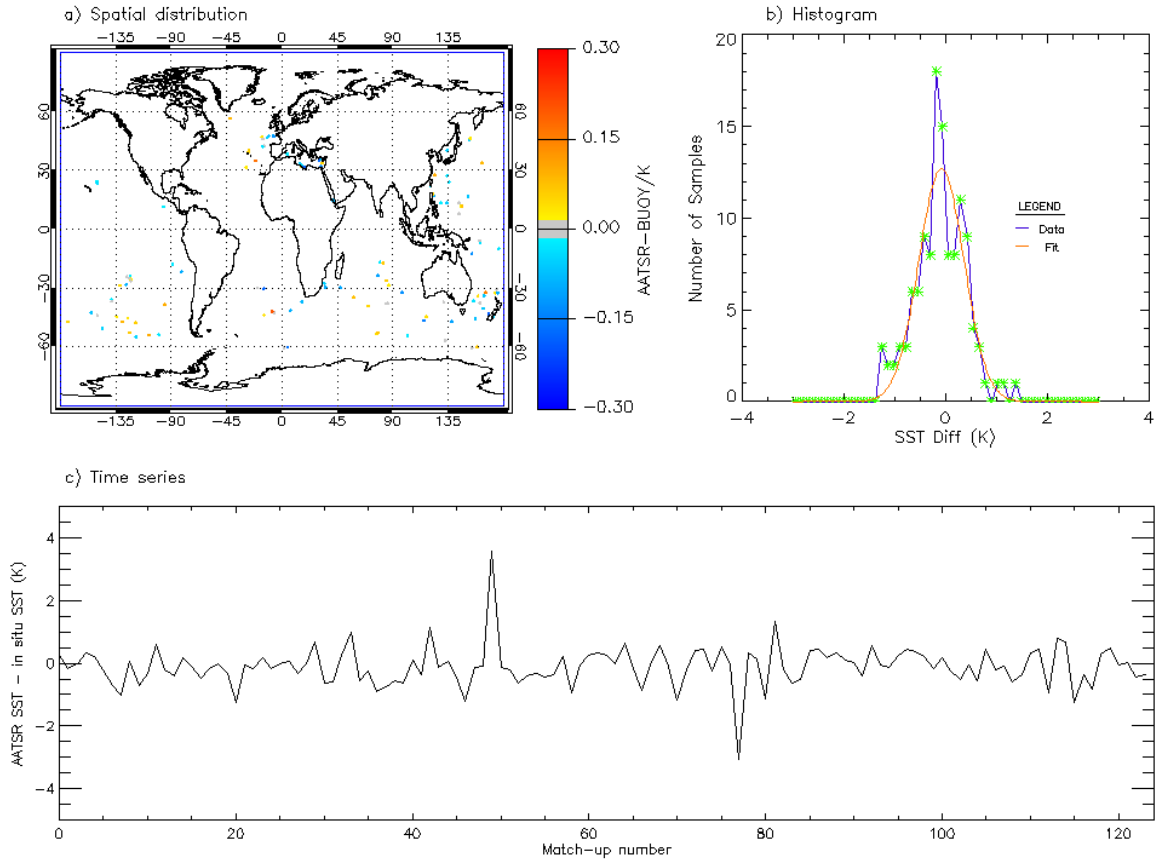

Figure 3-57: Spatial distribution, histogram and time series of Case 8 match-ups, 3-channel retrieval, TL_3 < D-N < TU_3, wind speed > 6 m^{-1}

The statistics for the Case 8 match-ups are given in Table 3-58. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-58: Statistics for Case 8 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	125	-0.100	0.65	-0.090	0.50
Moored only	46	-0.070	0.52	-0.120	0.47
Ships only	1682	-0.170	1.46	-0.151	1.25
TTP* only	14	-0.216	0.22	-0.242	0.23

*TTP = TAO/TRITON/PIRATA moored buoys

3.5.17 Case 9: 3-channel retrieval, D-N < TL_3, wind speed < 6 m^{-1}

Analysis of the ATSR-1 MDB did not produce any match-ups in this case.

3.5.18 Case 10: 3-channel retrieval, D-N < TL_3, wind speed > 6 m^{-1}

Analysis of the ATSR-1 MDB did not produce any match-ups in this case.

3.5.19 Case 11: 3-channel retrieval, D-N > TU_3, wind speed < 6 m^{-1}

Figure 3-58 shows a) the spatial distribution of Case 11 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between ATSR-1 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

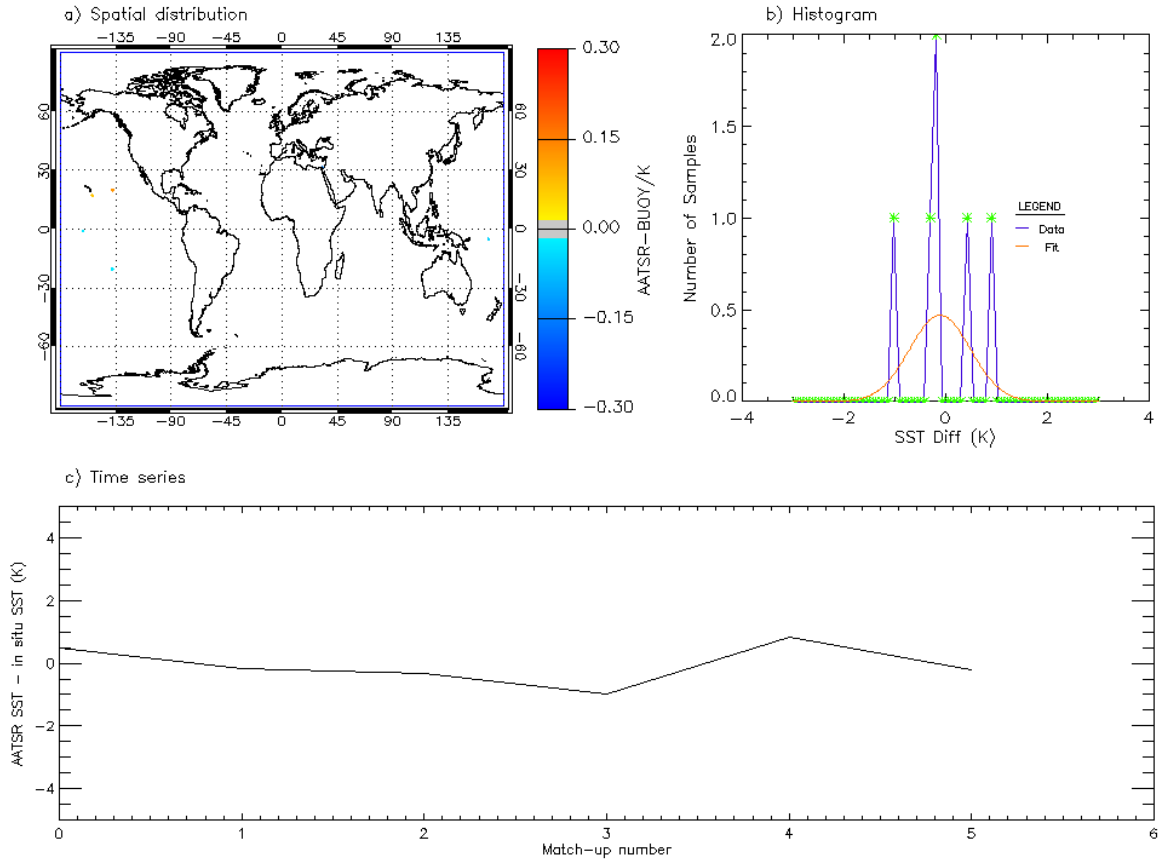

Figure 3-58: Spatial distribution, histogram and time series of Case 11 match-ups, 3-channel retrieval, D-N > TU_3, wind speed < 6 m^{-1}

The statistics for the Case 11 match-ups are given in Table 3-59. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-59: Statistics for Case 11 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	6	-0.061	0.64	-0.177	0.70
Moored only	8	+0.254	0.69	+0.126	0.74
Ships only	149	+0.111	1.46	+0.170	1.42
TTP* only	12	-0.023	0.27	-0.016	0.25

*TTP = TAO/TRITON/PIRATA moored buoys

3.5.20 Case 12: 3-channel retrieval, D-N > TU_3, wind speed > 6 m^{-1}

Figure 3-59 shows a) the spatial distribution of Case 12 match-ups, b) the histogram of the match-ups (together with a fitted Gaussian), and c) a time series of the differences between ATSR-1 and the in situ data. As noted earlier, a 3-sigma filter is applied to the data before the statistical analysis is carried out.

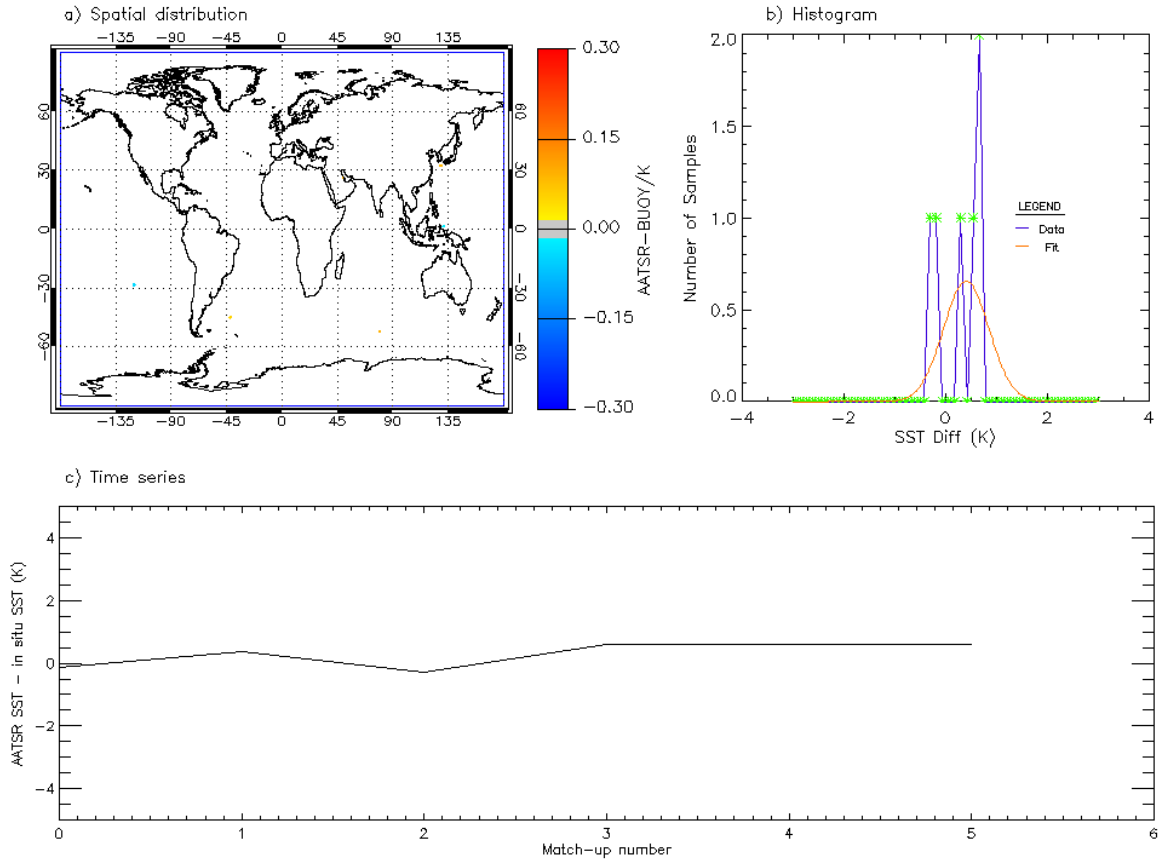

Figure 3-59: Spatial distribution, histogram and time series of Case 12 match-ups, 3-channel retrieval, D-N < TU_3, wind speed > 6 m^{-1}

The statistics for the Case 12 match-ups are given in Table 3-60. The statistics are given for surface drifting buoys only, moored buoys only and ships only.

Table 3-60: Statistics for Case 12 match-ups.

Dataset	Statistics				
	Number	Bias (°C)	Sigma (°C)	Median (°C)	Robust Sigma (°C)
Drifters only	6	+0.291	0.41	+0.474	0.52
Moored only	3	+0.094	0.57	+0.332	0.88
Ships only	159	+0.107	1.32	+0.120	1.25
TTP* only	1	-0.201	-	-	-

*TTP = TAO/TRITON/PIRATA moored buoys

3.5.21 Summary of the Analysis

Table 3-62 summarises the match-up statistics for all 12 cases (including day and night time 2-channel cases). Additional match-up statistics are provided in tables 3-62 to 3-70, where the wind speed dependency has been removed. Inspection of tables 3-37 to 3-43 highlights the following:

- The total number of match-ups to surface drifting buoys is exceedingly low. This is due to the low number of drifting buoys available during the ATSR-1 period.
- Again, there is little if any wind speed dependence observed, compared to the Medspiration AATSR MDB [AD2].
- The calculated 3-channel biases are very similar to the later missions, with larger variances, even with the robust statistics.

As for the other sensors, the ATSR-1 SSTs are skin SSTs and so an adjustment of + 0.17 K should be added to all biases when converting tables 3-37 to 3-43 into the SSES bias values.

Table 3-61: Summary of validation statistics for all stratification cases

Data Set		Statistics				
		Number	Mean (ºC)	Sigma (ºC)	Median (ºC)	Robust Sigma (ºC)
Case 1 Day	Drifters only	2734	-0.007	0.88	+0.030	0.68
	Moored only	2787	-0.012	0.84	+0.018	0.74
	Ships only	20197	-0.065	1.58	-0.048	1.39
	TTP* only	1250	+0.034	0.54	+0.018	0.53
Case 2 Day	Drifters only	2156	+0.054	0.79	+0.070	0.67
	Moored only	765	-0.102	0.97	-0.055	0.74
	Ships only	16193	-0.098	1.51	-0.090	1.34
	TTP* only	300	-0.017	0.56	-0.005	0.56
Case 3 Day	Drifters only	108	-0.786	0.67	-0.755	0.67
	Moored only	81	-1.191	0.85	-1.130	0.83
	Ships only	1065	-0.595	1.52	-0.581	1.40
	TTP* only	319	-0.507	0.53	-0.480	0.52
Case 4 Day	Drifters only	75	-0.818	0.72	-0.755	0.72
	Moored only	13	-1.328	1.12	-1.292	1.11
	Ships only	649	-0.781	1.44	-0.761	1.39
	TTP* only	68	-0.529	0.60	-0.429	0.53
Case 5 Day	Drifters only	128	+0.094	2.11	+0.521	0.98
	Moored only	120	+0.782	1.32	+0.778	1.05
	Ships only	1371	+0.364	1.88	+0.452	1.63
	TTP* only	25	+0.510	0.83	+0.331	0.81
Case 6 Day	Drifters only	130	-0.457	2.83	+0.190	0.99
	Moored only	35	+0.245	2.60	+0.635	1.28
	Ships only	1312	+0.228	1.88	+0.280	1.64
	TTP* only	13	+0.557	0.80	+0.410	0.79
Case 1 Night	Drifters only	1211	-0.069	0.83	-0.029	0.65
	Moored only	1169	-0.093	0.87	-0.051	0.73
	Ships only	7786	-0.137	1.59	-0.100	1.38
	TTP* only	740	-0.062	0.52	-0.082	0.52
Case 2 Night	Drifters only	1084	-0.007	0.84	+0.001	0.65
	Moored only	376	-0.183	0.90	-0.129	0.70
	Ships only	6494	-0.126	1.45	-0.090	1.32
	TTP* only	180	-0.106	0.61	-0.100	0.60
Case 3 Night	Drifters only	52	-0.746	0.71	-0.681	0.70
	Moored only	30	-1.203	0.86	-1.232	0.78
	Ships only	422	-0.573	1.54	-0.595	1.49
	TTP* only	189	-0.576	0.52	-0.560	0.52

Data Set		Statistics				
		Number	Mean (ºC)	Sigma (ºC)	Median (ºC)	Robust Sigma (ºC)
Case 4 Night	Drifters only	36	-0.857	0.78	-0.735	0.77
	Moored only	7	-1.863	0.97	-1.708	1.02
	Ships only	284	-0.740	1.45	-0.750	1.37
	TTP* only	38	-0.670	0.59	-0.558	0.56
Case 5 Night	Drifters only	50	-0.308	2.84	+0.522	1.30
	Moored only	48	+0.970	1.01	+0.988	0.84
	Ships only	398	+0.475	1.87	+0.531	1.60
	TTP* only	8	+1.025	1.04	+0.858	1.14
Case 6 Night	Drifters only	85	-1.361	4.18	+0.120	1.10
	Moored only	9	-0.970	4.52	+0.332	0.86
	Ships only	401	+0.432	1.95	+0.510	1.77
	TTP* only	3	+0.473	1.42	+0.018	1.73
Case 7	Drifters only	115	-0.098	0.93	-0.111	0.48
	Moored only	171	-0.060	0.50	-0.056	0.46
	Ships only	1524	-0.172	1.42	-0.150	1.25
	TTP* only	42	-0.205	0.38	-0.165	0.35
Case 8	Drifters only	125	-0.100	0.65	-0.090	0.50
	Moored only	46	-0.070	0.52	-0.120	0.47
	Ships only	1682	-0.170	1.46	-0.151	1.25
	TTP* only	14	-0.216	0.22	-0.242	0.23
Case 9	Drifters only	-	-	-	-	-
	Moored only	-	-	-	-	-
	Ships only	-	-	-	-	-
	TTP* only	-	-	-	-	-
Case 10	Drifters only	-	-	-	-	-
	Moored only	-	-	-	-	-
	Ships only	-	-	-	-	-
	TTP* only	-	-	-	-	-
Case 11	Drifters only	6	-0.061	0.64	-0.177	0.70
	Moored only	8	+0.254	0.69	+0.126	0.74
	Ships only	149	+0.111	1.46	+0.170	1.42
	TTP* only	12	-0.023	0.27	-0.016	0.25
Case 12	Drifters only	6	+0.291	0.41	+0.474	0.52
	Moored only	3	+0.094	0.57	+0.332	0.88
	Ships only	159	+0.107	1.32	+0.120	1.25
	TTP* only	1	-0.201	-	-	-

*TTP = TAO/TRITON/PIRATA moored buoys

Table 3-62: Statistics for day time 2-channel retrieval, $TL_2 < D\text{-}N < TU_2$ (combining cases 1 and 2)

Dataset	Statistics				
	Number	Mean (°C)	Sigma (°C)	Median (°C)	Robust Sigma(°C)
Drifters only	4890	+0.022	0.84	+0.049	0.67
Moored only	3552	-0.032	0.87	0.000	0.74
Ships only	36390	-0.080	1.55	-0.061	1.37
TTP* only	1550	+0.024	0.54	+0.015	0.54

*TTP = TAO/TRITON/PIRATA moored buoys

Table 3-63: Statistics for day time 2-channel retrieval, $D\text{-}N < TL_2$ (combining cases 3 and 4)

Dataset	Statistics				
	Number	Mean (°C)	Sigma (°C)	Median (°C)	Robust Sigma(°C)
Drifters only	183	-0.814	0.71	-0.760	0.70
Moored only	94	-1.210	0.89	-1.131	0.86
Ships only	1714	-0.664	1.49	-0.660	1.40
TTP* only	387	-0.510	0.54	-0.452	0.52

*TTP = TAO/TRITON/PIRATA moored buoys

Table 3-64: Statistics for day time 2-channel retrieval, $D\text{-}N > TU_2$ (combining cases 5 and 6)

Dataset	Statistics				
	Number	Mean (°C)	Sigma (°C)	Median (°C)	Robust Sigma(°C)
Drifters only	28	-0.076	2.22	+0.428	1.00
Moored only	155	+0.778	1.36	+0.729	1.09
Ships only	2683	+0.303	1.88	+0.361	1.64
TTP* only	38	+0.526	0.81	+0.344	0.79

*TTP = TAO/TRITON/PIRATA moored buoys

Table 3-65: Statistics for night time 2-channel retrieval, $TL_2 < D\text{-}N < TU_2$ (combining cases 1 and 2)

Dataset	Statistics				
	Number	Mean (°C)	Sigma (°C)	Median (°C)	Robust Sigma(°C)
Drifters only	2295	-0.037	0.82	-0.012	0.65
Moored only	1545	-0.117	0.88	-0.070	0.72
Ships only	14280	-0.129	1.52	-0.091	1.35
TTP* only	920	-0.065	0.54	-0.082	0.54

*TTP = TAO/TRITON/PIRATA moored buoys

Table 3-66: Statistics for night time 2-channel retrieval, D-N < TL_2 (combining cases 3 and 4)

Dataset	Statistics				
	Number	Mean (°C)	Sigma (°C)	Median (°C)	Robust Sigma(°C)
Drifters only	88	-0.792	0.74	-0.711	0.72
Moored only	37	-1.332	0.90	-1.266	0.84
Ships only	706	-0.640	1.51	-0.672	1.44
TTP* only	227	-0.599	0.54	-0.560	0.54

*TTP = TAO/TRITON/PIRATA moored buoys

Table 3-67: Statistics for night time 2-channel retrieval, D-N > TU_2 (combining cases 5 and 6)

Dataset	Statistics				
	Number	Mean (°C)	Sigma (°C)	Median (°C)	Robust Sigma(°C)
Drifters only	135	-0.865	3.56	+0.350	1.18
Moored only	57	+0.879	1.67	+0.980	0.87
Ships only	799	+0.453	1.91	+0.522	1.68
TTP* only	11	+0.875	1.10	+0.358	1.27

*TTP = TAO/TRITON/PIRATA moored buoys

Table 3-68: Statistics for 3-channel retrieval, TL_3 < D-N < TU_3 (combining cases 7 and 8)

Dataset	Statistics				
	Number	Mean (°C)	Sigma (°C)	Median (°C)	Robust Sigma(°C)
Drifters only	240	-0.099	0.79	-0.105	0.49
Moored only	217	-0.062	0.50	-0.088	0.47
Ships only	3206	-0.169	1.44	-0.150	1.25
TTP* only	56	-0.188	0.32	-0.181	0.30

*TTP = TAO/TRITON/PIRATA moored buoys

Table 3-69: Statistics for 3-channel retrieval, D-N < TL_3 (combining cases 9 and 10)

Dataset	Statistics				
	Number	Mean (°C)	Sigma (°C)	Median (°C)	Robust Sigma(°C)
Drifters only	-	-	-	-	-
Moored only	8	-0.785	0.99	-0.371	1.17
Ships only	35	-0.767	1.22	-0.850	1.27
TTP* only	-	-	-	-	-

*TTP = TAO/TRITON/PIRATA moored buoys

Table 3-70: Statistics for 3-channel retrieval, D-N > TU_3 (combining cases 11 and 12)

Dataset	Statistics				
	Number	Mean (°C)	Sigma (°C)	Median (°C)	Robust Sigma(°C)
Drifters only	12	+0.115	0.55	+0.108	0.57
Moored only	11	+0.210	0.63	+0.301	0.66
Ships only	308	+0.109	1.38	+0.160	1.33
TTP* only	13	-0.037	0.26	-0.040	0.25

*TTP = TAO/TRITON/PIRATA moored buoys

4 RECOMMENDED SSES SCHEME FOR ATSR-1, ATSR-2 AND AATSR

This section summarises the recommended SSES schemes for the (A)ATSR L2P reprocessing project, which should be included in the L2P files.

4.1 Summary of scheme

The analysis of the L2P AATSR MDB has indicated that little if any improvement is seen in the quality of the SSES for AATSR compared to Medspiration, despite using in situ data with improved QC such as ICOADS. The reason for this observation is not clear and is currently being investigated. Furthermore, attempts to provide stable temporally and spatially varying SSES have, so far, not been very successful and require further analysis (see later).

Consequently, the recommended scheme for AATSR (and therefore ATSR-1 and ATSR-2) will be:

- To use the current 12-level stratification scheme, with static bias and standard deviation values for each level for the archive (A)ATSR products, and no wind speed dependency
- To use the existing statistics from Medspiration for AATSR NRT products

As stated earlier, it is recommended that further research be done on the spatial and temporal variations of the SSES, to better quantify their benefits. However, this is likely to be a very time consuming process, and so to avoid delays to the L2P project, it should be continued offline.

It is very important to note that we are seeking benefits of the order of 0.1 to 0.2 K, and that the 12-level stratification with static bias and standard deviation provides data of significantly higher quality than that available from any other SST data set.

If, and when, significant benefits are found in the future, they will be recommended for adoption via the AATSR Quality Working Group (QWG).

4.2 Methodology

The SSES scheme for ATSR-1, ATSR-2 and AATSR is based on a 12-level stratification of the data set, with static bias and standard deviation values for each level; each level is also assigned a quality flag (or confidence value), which in the GDS is defined as the Proximity Confidence Value. The scheme is only applied to pixels where both the forward view and nadir view are cloud free. Consequently, the L2P data set will not contain nadir-only data that do not have a corresponding dual-view retrieval.

The 12-level stratification of the (A)ATSR data is based on:

1 The number of channels in the SST retrieval, either
   - 2-channel, or
   - 3-channel

2 The value of the dual-view minus nadir-only SST difference (or D-N) compared to a set of calculated thresholds [AD1], called T_{Un} and T_{Ln}, where T_U is an upper threshold and T_L is a lower threshold; n indicates the number of channels in the SST retrieval from step 1
   - D-N < T_{Ln}
   - T_{Ln} < D-N < T_{Un}
   - D-N > T_{Un}

3 The wind speed, being either
   - < 6 ms^{-1}, or
   - > 6 ms^{-1}

A more complete description of the scheme is given in AD1, AD2 and Section 3 of this document.

Therefore, to apply the SSES scheme to an (A)ATSR orbit requires:

1. Selecting all valid SST pixels within the orbit, where both the forward and nadir view are cloud free. For the moment we are only outputting pixels where both the forward and nadir are clear as we do not have an SSES scheme to allow for nadir-only retrievals to be included in the L2P file.

2. Creating a land mask for the entire orbit.

3. Creating a mask to indicate which SST retrieval was used for the valid data from step 1, which can be either a dual-view 3-channel or dual-view 2-channel retrieval.

4. Obtaining the wind speed for valid SST pixel from the ancillary data.

5. Stratifying all valid SST pixels according to number of channels in the retrieval, the values of D-N compared to predefined thresholds, and whether the wind speed is < or > 6 ms^{-1}.

6. Assigning a bias, standard deviation and proximity confidence flag for each valid SST pixel (the SSES).

7. Outputting the SSES as part of the L2P format (A)ATSR file.

An example IDL program to produce SSES for an AATSR orbit file according to the logical flow detailed above is included later in Section 6. The same scheme can be applied to ATSR-1 and ATSR-2, but will require bias, standard deviation and quality flags specific to each sensor. These can be found as the output to WP 41, deliverable D4.1.

We now consider each step of the SSES methodology in more detail.

Select valid SST pixels where both the forward and nadir view are cloud free:
The test for valid dual-view SST retrieval requires checking the bits of the Level 2 NR confidence word, which is included in the DISTRIB_SST_CLOUD_LAND_MDS records. A summary of the Level 2 confidence word meaning is given below:

Bit	Meaning if Set
0	Nadir-only SST is valid
1	Nadir-only SST retrieval includes 3.7 micron channel
2	Dual-view SST is valid
3	Dual-view SST retrieval includes 3.7 micron channel
4	Pixel is over land
5	Nadir-view pixel is cloudy
6	Nadir-view pixel has blanking pulse
7	Nadir-view pixel is cosmetic fill
8	Forward view pixel is cloudy
9	Forward-view pixel has blanking pulse
10	Forward-view pixel is cosmetic fill
11	One or both views flagged cloudy by 1.6 microns test (day time only)
12	Cloud flagged by 11 micron/12 micron nadir-forward test
13	One or both views flagged cloudy by infra-red histogram test
14-15	

A valid clear-sky dual-view SST is found by analysing the confidence word and noting if bit 0 and bit 2 are set, and if bit 4, bit 5 and bit 8 are not set. This is in accordance with the guidelines in the AATSR product handbook and FAQ. If a valid clear-sky dual-view retrieval is found then this should be recorded in a running total of all valid dual-view clear-sky coincidences.

The L2P data produced within this project will not contain valid nadir-only SSTs that have no coincident dual-view SSTs. To include these data in the future, then a valid nadir-only SST is found by analysing the confidence word and noting if bit 0 is set, and if bit 4 and bit 5 are not set.

Create a land mask:
A mask to indicate land pixels is required. This is obtained by checking if bit 4 of the Level 2 confidence word has been set for all pixels in the orbit file.

Create a retrieval type mask:
A flag to indicate the type of SST retrieval should be created. There are four possible SST retrievals, which are:

1. Dual-view 2-channel

   Found by checking if bit 1 and bit 3 of the Level 2 confidence word have not been set for pixels with a valid clear-sky dual-view SST.

2. Dual-view 3-channel

   Found by checking if bit 1 and bit 3 of the Level 2 confidence word have been set for pixels with a valid clear-sky dual-view SST.

3. Nadir-only 2-channel

   Found by checking if bit 1 and bit 3 of the Level 2 confidence word have not been set for pixels with a valid nadir-only SST but not a valid dual-view SST.

4. Nadir-only 3-channel

   Found by checking if bit 1 and bit 3 of the Level 2 confidence word have been set for pixels with a valid nadir-only SST but not a valid dual-view SST.

Obtain the wind speed for each pixel:
The wind speed for each pixel is required. This should be obtained from the ancillary data field that is required for each pixel in the file. If no wind speed is available for a particular pixel then the _FillValue of -128 should be included.

Stratify all pixels for each orbit according to number of channels, D-N threshold and wind speed:
All valid clear-sky dual-view SSTs within each orbit file are stratified according to the number of channels in the retrieval, the value of D-N compared to a threshold and the value of the wind speed, if the wind speed is valid. The process is repeated for pixels with a valid SST but an invalid wind speed.

The stratification process can be summarised as:

Step 1: Select valid SST pixels with valid wind speeds.

Step 2: Split valid SST pixel with valid wind speeds into two subsets according to whether the SSTs retrieval was a three-channel retrieval or not.

Step 3: For each subset from step 2, further subdivide the data based on the dual-view minus nadir-only SST values (D-N) for each pixel, according to the following:

D-N Stratification for Step 3	
If 2-channel Retrieval	**If 3-channel Retrieval**
$TL_2 <$ **D-N** $< TU_2$	$TL_3 <$ **D-N** $< TU_3$
D-N $< TL_2$	**D-N** $< TL_3$
D-N $> TU_2$	**D-N** $> TU_3$

The values of the thresholds for AATSR are:

- TU_2 = + 0.04
- TL_2 = - 1.53
- TU_3 = + 0.51
- TL_3 = - 0.51

The values of the thresholds for ATSR-2 are:

- TU_2 = + 0.39
- TL_2 = - 1.45
- TU_3 = + 0.61
- TL_3 = - 0.63

The values of the thresholds for ATSR-1 are:

- TU_2 = + 1.24
- TL_2 = - 0.95
- TU_3 = + 1.15
- TL_3 = - 0.38

We are then left with 6 subsets of our original data from step 1.

Step 4: Each of the 6 subsets from step 3 is then further subdivided according to whether the wind speed value is < 6 ms-1 or > 6 ms-1. This results in our final 12-level stratification of the data set.

Step 5: Select valid SST pixels with invalid wind speeds.

Step 6: Repeat step 2 for the pixels selected in step 5.

Step 7: Repeat step 3 for the pixels selected from step 5 and step 6.

Assign a bias, standard deviation and proximity confidence flag for each pixel:

Once each valid SST within the orbit has been classified according to the 12-level stratification, the next step is assign the static bias, standard deviation and proximity confidence value.

As detailed earlier in Section 4.1, it is recommended that the AATSR SSES are those derived for Medspiration and not those presented in Section 3.3.14, owing to the poor wind speed dependency. The Medspiration AATSR SSES are defined in AD2.

The SSES values for AATSR are:

Stratification Case	Summary of criteria			Bias	Standard Deviation	Proximity Confidence Value
Case 1:	2-channel	$TL_2 < \mathbf{D\text{-}N} < TU_2$	Wind < 6ms^{-1}	+0.20	0.33	5
Case 2:	2-channel	$TL_2 < \mathbf{D\text{-}N} < TU_2$	Wind > 6ms^{-1}	+0.20	0.33	5
Case 3:	2-channel	$\mathbf{D\text{-}N} < TL_2$	Wind < 6ms^{-1}	-0.41	0.71	3
Case 4:	2-channel	$\mathbf{D\text{-}N} < TL_2$	Wind > 6ms^{-1}	-0.41	0.71	3
Case 5:	2-channel	$\mathbf{D\text{-}N} > TU_2$	Wind < 6ms^{-1}	+0.71	0.64	3
Case 6:	2-channel	$\mathbf{D\text{-}N} > TU_2$	Wind > 6ms^{-1}	+0.71	0.64	3
Case 7:	3-channel	$TL_3 < \mathbf{D\text{-}N} < TU_3$	Wind < 6ms^{-1}	+0.11	0.32	5
Case 8:	3-channel	$TL_3 < \mathbf{D\text{-}N} < TU_3$	Wind > 6ms^{-1}	+0.11	0.32	5
Case 9:	3-channel	$\mathbf{D\text{-}N} < TL_3$	Wind < 6ms^{-1}	-0.65	0.49	4
Case 10:	3-channel	$\mathbf{D\text{-}N} < TL_3$	Wind > 6ms^{-1}	-0.65	0.49	4
Case 11:	3-channel	$\mathbf{D\text{-}N} > TU_3$	Wind < 6ms^{-1}	+0.69	0.32	4
Case 12:	3-channel	$\mathbf{D\text{-}N} > TU_3$	Wind > 6ms^{-1}	+0.69	0.32	4

The SSES values for ATSR-2 are:

Stratification Case	Summary of criteria			Bias	Standard Deviation	Proximity Confidence Value
Case 1:	2-channel	$TL_2 < \mathbf{D\text{-}N} < TU_2$	Wind < 6ms^{-1}	+0.07	0.43	5
Case 2:	2-channel	$TL_2 < \mathbf{D\text{-}N} < TU_2$	Wind > 6ms^{-1}	+0.07	0.43	5
Case 3:	2-channel	$\mathbf{D\text{-}N} < TL_2$	Wind < 6ms^{-1}	-0.43	0.78	3
Case 4:	2-channel	$\mathbf{D\text{-}N} < TL_2$	Wind > 6ms^{-1}	-0.43	0.78	3
Case 5:	2-channel	$\mathbf{D\text{-}N} > TU_2$	Wind < 6ms^{-1}	+0.24	0.83	3
Case 6:	2-channel	$\mathbf{D\text{-}N} > TU_2$	Wind > 6ms^{-1}	+0.24	0.83	3
Case 7:	3-channel	$TL_3 < \mathbf{D\text{-}N} < TU_3$	Wind < 6ms^{-1}	+0.06	0.35	5
Case 8:	3-channel	$TL_3 < \mathbf{D\text{-}N} < TU_3$	Wind > 6ms^{-1}	+0.06	0.35	5
Case 9:	3-channel	$\mathbf{D\text{-}N} < TL_3$	Wind < 6ms^{-1}	-0.61	0.57	4
Case 10:	3-channel	$\mathbf{D\text{-}N} < TL_3$	Wind > 6ms^{-1}	-0.61	0.57	4
Case 11:	3-channel	$\mathbf{D\text{-}N} > TU_3$	Wind < 6ms^{-1}	+0.51	0.39	4
Case 12:	3-channel	$\mathbf{D\text{-}N} > TU_3$	Wind > 6ms^{-1}	+0.51	0.39	4

The SSES values for ATSR-1 are:

Stratification Case	Summary of criteria			Bias	Standard Deviation	Proximity Confidence Value
Case 1:	2-channel	TL_2 < **D-N** < TU_2	Wind < 6ms^{-1}	+0.16	0.65	5
Case 2:	2-channel	TL_2 < **D-N** < TU_2	Wind > 6ms^{-1}	+0.16	0.65	5
Case 3:	2-channel	**D-N** < TL_2	Wind < 6ms^{-1}	-0.54	0.72	3
Case 4:	2-channel	**D-N** < TL_2	Wind > 6ms^{-1}	-0.54	0.72	3
Case 5:	2-channel	**D-N** > TU_2	Wind < 6ms^{-1}	+0.52	1.18	3
Case 6:	2-channel	**D-N** > TU_2	Wind > 6ms^{-1}	+0.52	1.18	3
Case 7:	3-channel	TL_3 < **D-N** < TU_3	Wind < 6ms^{-1}	+0.07	0.49	5
Case 8:	3-channel	TL_3 < **D-N** < TU_3	Wind > 6ms^{-1}	+0.07	0.49	5
Case 9:	3-channel	**D-N** < TL_3	Wind < 6ms^{-1}	-	-	2
Case 10:	3-channel	**D-N** < TL_3	Wind > 6ms^{-1}	-	-	2
Case 11:	3-channel	**D-N** > TU_3	Wind < 6ms^{-1}	+0.28	0.57	4
Case 12:	3-channel	**D-N** > TU_3	Wind > 6ms^{-1}	+0.28	0.57	4

For valid SST pixels identified from step 5, step 6 and step 7, with invalid wind speed data, it will not be possible to distinguish case 7 from case 8, case 9 from case 10 and case 11 from case 12. For these pixels, the bias should be set as the mean between the two options, the higher of the standard deviation options is selected and, where the proximity confidence value is 5, it is reduced to 4.

Output the SSES as part of the L2P format (A)ATSR file:

The final step is to output the SSES as part of the L2P file. The bias, standard deviation and proximity confidence values take their normal field names, as defined in the GDS [AD3]. The L2P file will require one experimental field to be added to output the D-N SST difference, and the modification of the confidence flag to accommodate the retrieval type mask.

The experimental field will require two additional bytes to be added to the L2P file, and should be included as a new variable in the NetCDF format files according to the following specification:

Name	Comment
SHORT *atsr_dual_nadir_sst_difference* (time, nj, ni) [a,b]	Difference between dual-view and nadir-only SST retrievals. Ranges from -327.67 °C to +327.67 °C [c] Precision of 0.01 °C

[a] This is an experimental field and is not defined in the GDS. The name is not likely to be CF compliant as it is too specialised, but will be verified at the next GHRSST-PP science team meeting.

[b] It is assumed that the dimensions of the experimental fields will be the same as the other variables within the L2P file.

[c] The current range of *atsr_dual_nadir_sst_difference* is set to allowable limits of short word integer with precision of 0.01 °C until a more realistic range is calculated.

The following attributes should be included for the new variable:

- *atsr_dual_nadir_sst_difference:*
  - long_name = atsr dual minus nadir sst difference
  - units = kelvin
  - _FillValue = -32768
  - add_offset = 0.00
  - scale_factor = 0.01
  - coordinates = lon lat
  - valid_min = -32767
  - valid_max = 32768

To avoid adding a further byte of data to each L2P files, at the suggestion of Jean François Piolle (Ifremer), the existing confidence flag variable will be reformulated for (A)ATSR to accommodate the retrieval type mask. The current confidence flag has several bits that are solely relevant to microwave SSTs, which will be redefined. The metadata description for the confidence flag variable within the L2P file will now be for (A)ATSR:

b0 = type of retrieval in sea_surface_temperature variable (0: dual-view, 1: nadir-only)
b1 = retrieval in sea_surface_temperature variable used 3.7 micron channel (0: No, 1: Yes)
b2 = spare
b3 = spare
b4 = spare
b5 = spare
b6: 1 = L2 native bias and standard deviation;
b7: 1 = L2 native confidence value

Note: b5, the sun glint flag, is only available from (A)ATSR Level 1b data so we cannot set this for (A)ATSR; b6 and b7 keep their original definitions.

So, for each pixel you set b1 if the 3.7 channel was used in the retrieval; b0 will always be set to zero at this stage as we are only including dual-view SSTs in the file. In the future, b0 would be set to 1 if a nadir-only SST is included, with of course a zero D-N difference.

The above definition will be submitted to the GDS 2.0 specification, and Jean François Piolle is making the same changes to the current Medspiration product chain.

5 SUMMARY AND CONCLUSIONS

An investigation into the temporal and spatial dependency of the Medspiration SSES scheme for AATSR has been carried out, and SSES values have been determined for all three sensors in the (A)ATSR series.

The results of the temporal and spatial analysis indicate that some small scale spatial features are seen, which may be accounted for in a future refinement of the SSES. These are:

- The inclusion of the D2-D3 latitudinal bias
- The inclusion of an additional high latitude correction once the error source is understood.

However, it is likely that a lot of the observed spatial differences are due to natural variations in the skin effect, which is not currently corrected for in the MDB, and the simplistic approach of the stratification at $6ms^{-1}$ is used instead.

Consequently, it is recommended that in the future, the MDB is modified to allow for an improved skin effect adjustment, which also allows for diurnal heating.

Therefore, it is recommended that the current Medspiration AATSR SSES scheme based on the D-N SST difference is used for processing all data within the (A)ATSR L2P project, using the SSES given in this report.

6 EXAMPLE IDL FILE

This section contains an example IDL program to output updated SSES. The program has one difference to the scheme detailed in this report, in that it uses the wind speed from the Medspiration L2P file corresponding to the N1 file being processed. The program was written to produce D1.2, the test data set for the Met Office.

```
;-------------------------------------------------------------------------
;                       PRO aatsr_SSES_example
;
;
;-------------------------------------------------------------------------
; AUTHOR:  Gary Corlett
; DATE:    January 2008
;
; Version 1.0 - 16/01/2008
; Version 1.1 - 23/01/2008 - modified to allow for nadir only SSTs to be included in the future
; Version 1.2 - 25/03/2008 - modified for final medspiration scheme
;
; ABOUT THE PROGRAM:
; This programme produces updated SSES for AATSR using the new UL method.
;
; The programme opens a NRT L2P file and then determines a land mask, a 3-channel mask and the dual-nadir SST difference.  The programme
; then reads the wind speed from the Medspiration data file.
;
; The programme ouputs the SSES in NetCDF.
;
; LIST OF VARIABLES:
;
; Inputs:
; none
;
; Outputs:
; The supplementary data file
;
; KEYWORDS:
; none
;
; ADDITIONAL PROCEDURES REQUIRED:
; read_header
; extract_data_set_v6
; geoloc_atsr
;
; LIMITATIONS:
; This program can only output a single orbit SSES file, and requires wind speed for each pixel. This example programme takes wind speed from the
; Medspiration L2P file.  If wind speed is not available then the bias is set as the mean between the two options, the high of the standard
; deviation options would be selected, and where the proximity confidence values is 5, it should be lowered to 4.
;
;-------------------------------------------------------------------------------

pro aatsr_SSES_example

;*****************************************************************************
; User defined variables and paths
n1_path = 'D:\WORK\L2P\aatsr_SSES\output\ForJFP\N1\'
med_path = 'D:\WORK\L2P\aatsr_SSES\output\ForJFP\Meds\'
out_path = 'D:\WORK\L2P\aatsr_SSES\output\ForJFP\'
do_nadir_only = 0       ; flag to indicate if nadir=only data should be included

;*****************************************************************************
; Do not modify code below this point
;*****************************************************************************

; Check all inputs/outputs are closed. Print start time to screen
close, /all
print, 'Started at: ', SYSTIME()
```

```
; Select N1 file
n1_file_select = dialog_pickfile(filter='*.N1.gz', path=n1_path)
n1_file = STRMID(n1_file_select, 64, 65, /REVERSE_OFFSET)

; Select L2P file equivalent to N1 file
med_file = STRMID(n1_file, 50, 8, /REVERSE_OFFSET)+'-ATS_NR_2P-EUR-L2P-'+STRMID(n1_file, 64, 62, /REVERSE_OFFSET)+'-v01.nc'

; Check L2P files exists - if not then stop
file_exist = FILE_SEARCH(med_path+med_file, count=count)
if count eq 0 then stop

;Open data file
ext=STRMID(n1_file, 0, 2, /REVERSE_OFFSET)
ext=STRLOWCASE(ext)
IF (ext EQ 'n1') THEN OPENR, l2lun, n1_path+n1_file,/get_lun ELSE OPENR, l2lun, n1_path+n1_file, /get_lun, /compress

;Read the MPH, SPH and DSDs - store in DSinfo.  Note flag MET must be set earlier in program.
read_header, n1_file, l2lun, DSinfo, met, corrupt_flag, version

; retrun if AATSR file is corrupt
IF corrupt_flag EQ 1 THEN retrun

;get geolocation ADS
extract_data_set_v6, l2lun, DSinfo, 'GEOLOCATION_ADS            ', 0, 0, met, geo

; geolocate
geoloc_atsr, geo, grid_geo, /corners

; Extract corner coordinates and delete arrays
aatsr_lat_grid = grid_geo.corner_lats/1e6
aatsr_lon_grid = grid_geo.corner_lons/1e6
geo=0
grid_geo = 0

; read MDS
extract_data_set_v6, l2lun, DSinfo, 'DISTRIB_SST_CLOUD_LAND_MDS  ', 0, 0, met, data

; Close data file
close, l2lun
free_lun, l2lun

; Now check data against flags.
; Need to check the nadir/dual valid flag, land flag and nadir/forward cloudy.
dual_sst = data.comb_field
nadir_sst = data.nad_field
dual_check = (2L^0 + 2L^2)+2L^4+(2L^5+2L^8)
nadir_check = (2L^0)+2L^4+(2L^5)
dual_ok=(2L^0 + 2L^2)
nadir_ok=2L^0
index=WHERE((data.conf_wd AND dual_check) NE dual_ok, count)
IF count GT 0 THEN dual_sst[index]=-32768
if do_nadir_only eq 1 then index=WHERE((data.conf_wd AND nadir_check) NE nadir_ok, count)
IF count GT 0 THEN nadir_sst[index]=-32768
flags = data.conf_wd
data=0
index = 0
; Set all "valid" SSTs below -2 celcius to _FillValue
index = where(dual_sst ne -32768 and dual_sst lt 27315, count)
if count gt 0 then dual_sst[index] = -32768
index = where(nadir_sst ne -32768 and nadir_sst lt 27315, count)
if count gt 0 then nadir_sst[index] = -32768
index = where(dual_sst ne -32768 and nadir_sst eq -32768, count)
if count gt 0 then dual_sst[index] = -32768
index = 0

; Select medpiration file for wind speed
cd, med_path

; Open Medspiration NetCDF file
id = NCDF_OPEN(med_file)
```

```
; Read wind_speed data.  IDL cannot read signed integers, so need to convert to short integer
NCDF_VARGET, id, 'wind_speed', wind_speed
NCDF_ATTGET, id, 'wind_speed', 'add_offset', offset_WS
NCDF_ATTGET, id, 'wind_speed', 'scale_factor', scale_factor_WS
wind_speed = fix(wind_speed)
index = where(wind_speed ge 128, count)
if count gt 0 then wind_speed[index] = wind_speed[index] - 256
wind_speed_float = float(wind_speed)
index = where(wind_speed_float ne -128.0, count)
wind_speed_float[index] = (wind_speed_float[index]*scale_factor_WS) + offset_WS
wind_speed = 0
index = 0

; Close Medspiration NetCDF file
NCDF_CLOSE, id

; For some reason the Medspiration data files do not contain the last granule of data!!
; Add granule of blank data to wind speed
max_dim = ((size(wind_speed_float))[2]) - 1
wind_speed = dual_sst
wind_speed[*,*] = -128.0
wind_speed[*,0:max_dim] = wind_speed_float
wind_speed_float = 0

; Create land mask
land_mask = fix(flags)
land_mask(*,*) = -999.0
land_check = 2L^4
land_ok = 2L^4
index=WHERE((flags AND land_check) EQ land_ok, count)
if count gt 0 then land_mask[index] = 1.0

; Create retrieval type mask
retrieval_mask = fix(flags)
retrieval_mask(*,*) = -128.0
dual_three_check = 2L^1 + 2L^3
dual_three_ok=2L^1 + 2L^3
nadir_three_check = 2L^1
nadir_three_ok=2L^1

; Set retrieval type
; Dual 2-channel
index=WHERE(((flags AND dual_three_check) NE dual_three_ok) and dual_sst ne -32768.0, count)
if count gt 0 then retrieval_mask[index] = 0
; Dual 3-channel
index=WHERE(((flags AND dual_three_check) EQ dual_three_ok) and dual_sst ne -32768.0, count)
if count gt 0 then retrieval_mask[index] = 1
; Nadir 2-channel with no dual
index=WHERE(((flags AND nadir_three_check) NE nadir_three_ok) and nadir_sst ne -32768.0 and dual_sst eq -32768, count)
if count gt 0 then retrieval_mask[index] = 2
; Nadir 3-channel with no dual
index=WHERE(((flags AND nadir_three_check) EQ nadir_three_ok) and nadir_sst ne -32768.0 and dual_sst eq -32768, count)
if count gt 0 then retrieval_mask[index] = 3

; Convert SSTs
index=WHERE(dual_sst NE -32768., count)
dual_sst=temporary(FLOAT(dual_sst))
IF index[0] GT -1 THEN dual_sst[index]=dual_sst[index]/100.
index=WHERE(nadir_sst NE -32768., count)
nadir_sst=temporary(FLOAT(nadir_sst))
IF index[0] GT -1 THEN nadir_sst[index]=nadir_sst[index]/100.

; Calculate D-N difference
diff = dual_sst
diff(*,*) = -32768.0
index = where(dual_sst ne -32768.0)
diff(index) = dual_sst(index) - nadir_sst(index)

; Set up output fields for SSES
proximity_confidence = fix(flags)
proximity_confidence(*,*) = 1
```

```
SSES_bias_error = float(flags)
SSES_bias_error(*,*) = -128.0
SSES_standard_deviation_error = float(flags)
SSES_standard_deviation_error(*,*) = -128.0

; Define D-N thresholds
tu2 = 0.04
tl2 = -1.53
tu3 = 0.51
tl3 = -0.51

; Define SSES values
b1 = 0.23
b2 = 0.18
b3 = -0.44
b4 = -0.44
b5 = 0.78
b6 = 0.78
b7 = 0.04
b8 = 0.10
b9 = -0.77
b10 = -0.68
b11 = 0.59
b12 = 0.65
s1 = 0.39
s2 =0.34
s3 = 0.73
s4 = 0.73
s5 = 0.67
s6 = 0.67
s7 = 0.33
s8 = 0.33
s9 = 0.51
s10 = 0.42
s11 = 0.35
s12 = 0.32
c1 = 5
c2 =5
c3 = 3
c4 = 3
c5 = 3
c6 = 3
c7 = 5
c8 = 5
c9 = 4
c10 = 4
c11 = 4
c12 = 4

; Stratify data for SSES

; Valid wind speeds

; Case 1
index = where(retrieval_mask eq 0 and wind_speed ne -128 and wind_speed le 6.0 and diff ge tl2 and diff le tu2, count)
if count gt 0 then proximity_confidence[index] = c1
if count gt 0 then SSES_bias_error[index] = b1
if count gt 0 then SSES_standard_deviation_error[index] = s1
; Case 3
index = where(retrieval_mask eq 0 and wind_speed ne -128 and wind_speed le 6.0 and diff lt tl2, count)
if count gt 0 then proximity_confidence[index] = c3
if count gt 0 then SSES_bias_error[index] = b3
if count gt 0 then SSES_standard_deviation_error[index] = s3
; Case 5
index = where(retrieval_mask eq 0 and wind_speed ne -128 and wind_speed le 6.0 and diff gt tu2, count)
if count gt 0 then proximity_confidence[index] = c5
if count gt 0 then SSES_bias_error[index] = b5
if count gt 0 then SSES_standard_deviation_error[index] = s5
; Case 2
index = where(retrieval_mask eq 0 and wind_speed ne -128 and wind_speed gt 6.0 and diff ge tl2 and diff le tu2, count)
if count gt 0 then proximity_confidence[index] = c2
```

```
if count gt 0 then SSES_bias_error[index] = b2
if count gt 0 then SSES_standard_deviation_error[index] = s2
; Case 4
index = where(retrieval_mask eq 0 and wind_speed ne -128 and wind_speed gt 6.0 and diff lt tl2, count)
if count gt 0 then proximity_confidence[index] = c4
if count gt 0 then SSES_bias_error[index] = b4
if count gt 0 then SSES_standard_deviation_error[index] = s4
; Case 6
index = where(retrieval_mask eq 0 and wind_speed ne -128 and wind_speed gt 6.0 and diff gt tu2, count)
if count gt 0 then proximity_confidence[index] = c6
if count gt 0 then SSES_bias_error[index] = b6
if count gt 0 then SSES_standard_deviation_error[index] = s6
; Case 7
index = where(retrieval_mask eq 1 and wind_speed ne -128 and wind_speed le 6.0 and diff ge tl3 and diff le tu3, count)
if count gt 0 then proximity_confidence[index] = c7
if count gt 0 then SSES_bias_error[index] = b7
if count gt 0 then SSES_standard_deviation_error[index] = s7
; Case 9
index = where(retrieval_mask eq 1 and wind_speed ne -128 and wind_speed le 6.0 and diff lt tl3, count)
if count gt 0 then proximity_confidence[index] = c9
if count gt 0 then SSES_bias_error[index] = b9
if count gt 0 then SSES_standard_deviation_error[index] = s9
; Case 11
index = where(retrieval_mask eq 1 and wind_speed ne -128 and wind_speed le 6.0 and diff gt tu3, count)
if count gt 0 then proximity_confidence[index] = c11
if count gt 0 then SSES_bias_error[index] = b11
if count gt 0 then SSES_standard_deviation_error[index] = s11
; Case 8
index = where(retrieval_mask eq 1 and wind_speed ne -128 and wind_speed gt 6.0 and diff ge tl3 and diff le tu3, count)
if count gt 0 then proximity_confidence[index] = c8
if count gt 0 then SSES_bias_error[index] = b8
if count gt 0 then SSES_standard_deviation_error[index] = s8
; Case 10
index = where(retrieval_mask eq 1 and wind_speed ne -128 and wind_speed gt 6.0 and diff lt tl3, count)
if count gt 0 then proximity_confidence[index] = c10
if count gt 0 then SSES_bias_error[index] = b10
if count gt 0 then SSES_standard_deviation_error[index] = s10
; Case 12
index = where(retrieval_mask eq 1 and wind_speed ne -128 and wind_speed gt 6.0 and diff gt tu3, count)
if count gt 0 then proximity_confidence[index] = c12
if count gt 0 then SSES_bias_error[index] = b12
if count gt 0 then SSES_standard_deviation_error[index] = s12

; Invalid wind speeds

; Case 1 & Case 2
index = where(retrieval_mask eq 0 and wind_speed eq -128 and diff ge tl2 and diff le tu2, count)
if count gt 0 then proximity_confidence[index] = c1 - 1
if count gt 0 then SSES_bias_error[index] = (b1+b2)/2.0
if count gt 0 then SSES_standard_deviation_error[index] = s1
; Case 3 & Case 4
index = where(retrieval_mask eq 0 and wind_speed eq -128 and diff lt tl2, count)
if count gt 0 then proximity_confidence[index] = c3
if count gt 0 then SSES_bias_error[index] = b3
if count gt 0 then SSES_standard_deviation_error[index] = s3
; Case 5 & Case 6
index = where(retrieval_mask eq 0 and wind_speed eq -128 and diff gt tu2, count)
if count gt 0 then proximity_confidence[index] = c5
if count gt 0 then SSES_bias_error[index] = (b5+b6)/2.0
if count gt 0 then SSES_standard_deviation_error[index] = s5
; Case 7 & Case 8
index = where(retrieval_mask eq 1 and wind_speed eq -128 and diff ge tl3 and diff le tu3, count)
if count gt 0 then proximity_confidence[index] = c7 - 1
if count gt 0 then SSES_bias_error[index] = (b7+b8)/2.0
if count gt 0 then SSES_standard_deviation_error[index] = s7
; Case 9 & Case 10
index = where(retrieval_mask eq 1 and wind_speed eq -128 and diff lt tl3, count)
if count gt 0 then proximity_confidence[index] = c9
if count gt 0 then SSES_bias_error[index] = (b9+b10)/2.0
if count gt 0 then SSES_standard_deviation_error[index] = s9
; Case 11 & Case 12
```

```
index = where(retrieval_mask eq 1 and wind_speed eq -128 and diff gt tu3, count)
if count gt 0 then proximity_confidence[index] = c11 - 1
if count gt 0 then SSES_bias_error[index] = (b11+b12)/2.0
if count gt 0 then SSES_standard_deviation_error[index] = s11

; Add land mask to proximity confidence mask
index = where(land_mask eq 1.0, count)
if count gt 0 then proximity_confidence[index] = 0


; Create confidence flag
confidence_flag = byte(retrieval_mask)
confidence_flag[*,*] = 0
; First: dual-view 2-channel b0:0; b1:0
; No need to change array default value

; Second: dual-view 3-channel b0:0; b1:1
index = where(retrieval_mask eq 1, count)
if count gt 0 then confidence_flag[index] = 2^1

; Third: nadir-only 2-channel b0:1; b1:0
index = where(retrieval_mask eq 2, count)
if count gt 0 then confidence_flag[index] = 2^0

; Fourth: nadir-only 3-channel b0:1; b1:1
index = where(retrieval_mask eq 3, count)
if count gt 0 then confidence_flag[index] = 2^0 + 2^1

; Create output MDB file
;----------------------
; Note: Although IDL cannot read signed byte integers, it can write them providing they are stored as short integers but defined as byte to the output file!!!

output_filename = out_path+strmid(n1_file, 0, 62)+'-000001.nc'

;  Create the NetCDF output file
Id = NCDF_CREATE(output_filename,/CLOBBER)

; Write Global Attributes
NCDF_ATTPUT, Id, /GLOBAL, "title", "Supplementary L2P data file"
NCDF_ATTPUT, Id, /GLOBAL, "institution", "University of Leicester"
NCDF_ATTPUT, Id, /GLOBAL, "contact", "Gary Corlett (gkc1@le.ac.uk)"
NCDF_ATTPUT, Id, /GLOBAL, "creation_date", string(systime())
NCDF_ATTPUT, Id, /GLOBAL, "parent_N1_file", n1_file

; Create dimensions
Dim1   = NCDF_DIMDEF(Id,'time',1)
Dim2   = NCDF_DIMDEF(Id,'nj',((size(dual_sst))[2]))
Dim3   = NCDF_DIMDEF(Id,'ni',((size(dual_sst))[1]))

; Create variables and attributes to hold the data
 VarId  = NCDF_VARDEF(Id,'proximity_confidence', [Dim3,Dim2,dim1], /BYTE)
NCDF_ATTPUT, Id, VarId, 'long_name', 'proximity confidence value', /CHAR
NCDF_ATTPUT, Id, VarId, '_FillValue', -128, /BYTE
NCDF_ATTPUT, Id, VarId, 'coordinates', 'lon lat', /CHAR
NCDF_ATTPUT, Id, VarId, 'valid_min', -127, /BYTE
NCDF_ATTPUT, Id, VarId, 'valid_max', 127, /BYTE

VarId  = NCDF_VARDEF(Id,'confidence_flag', [Dim3,Dim2,dim1], /BYTE)
NCDF_ATTPUT, Id, VarId, 'long_name', 'AATSR confidence flag', /CHAR
NCDF_ATTPUT, Id, VarId, 'coordinates', 'lon lat', /CHAR
NCDF_ATTPUT, Id, VarId, 'comment1', 'b0: type of retrieval in sea_surface_temperature variable (0: dual-view, 1: nadir-only); b1: retrieval in sea_surface_temperature variable used 3.7 micron channel (0: No, 1:Yes)', /CHAR
NCDF_ATTPUT, Id, VarId, 'comment2', 'b2: spare; b3: spare; b4: spare; b5: spare; b6: 1 = L2 native bias and standard deviation; b7: 1 = L2 native bias and standard deviation', /CHAR

VarId  = NCDF_VARDEF(Id,'SSES_bias_error', [Dim3,Dim2,dim1], /BYTE)
NCDF_ATTPUT, Id, VarId, 'long_name', 'SSES bias error based on confidence flags', /CHAR
NCDF_ATTPUT, Id, VarId, 'units', 'kelvin', /CHAR
NCDF_ATTPUT, Id, VarId, '_FillValue', -128, /BYTE
NCDF_ATTPUT, Id, VarId, 'add_offset', 0.0, /FLOAT
```

```
NCDF_ATTPUT, Id, VarId, 'scale_factor', 0.01, /FLOAT
NCDF_ATTPUT, Id, VarId, 'coordinates', 'lon lat', /CHAR
NCDF_ATTPUT, Id, VarId, 'valid_min', -127, /BYTE
NCDF_ATTPUT, Id, VarId, 'valid_max', 127, /BYTE

VarId  = NCDF_VARDEF(Id,'SSES_standard_deviation_error', [Dim3,Dim2,dim1], /BYTE)
NCDF_ATTPUT, Id, VarId, 'long_name', 'SSES standard deviation error based on confidence flags', /CHAR
NCDF_ATTPUT, Id, VarId, 'units', 'kelvin', /CHAR
NCDF_ATTPUT, Id, VarId, '_FillValue', -128, /BYTE
NCDF_ATTPUT, Id, VarId, 'add_offset', 1.0, /FLOAT
NCDF_ATTPUT, Id, VarId, 'scale_factor', 0.01, /FLOAT
NCDF_ATTPUT, Id, VarId, 'coordinates', 'lon lat', /CHAR
NCDF_ATTPUT, Id, VarId, 'valid_min', -127, /BYTE
NCDF_ATTPUT, Id, VarId, 'valid_max', 127, /BYTE

; Note the following two fields are experimental fileds and are not defined in the GDS

VarId  = NCDF_VARDEF(Id,'atsr_dual_nadir_sst_difference', [Dim3,Dim2,dim1], /SHORT)
NCDF_ATTPUT, Id, VarId, 'long_name', 'atsr dual minus nadir sst difference', /CHAR
NCDF_ATTPUT, Id, VarId, 'units', 'kelvin', /CHAR
NCDF_ATTPUT, Id, VarId, '_FillValue', -32768, /SHORT
NCDF_ATTPUT, Id, VarId, 'add_offset', 0.0, /FLOAT
NCDF_ATTPUT, Id, VarId, 'scale_factor', 0.01, /FLOAT
NCDF_ATTPUT, Id, VarId, 'coordinates', 'lon lat', /CHAR
NCDF_ATTPUT, Id, VarId, 'valid_min', -32767, /SHORT
NCDF_ATTPUT, Id, VarId, 'valid_max', 32767, /SHORT

;  Leave definition mode and enter data write mode
NCDF_CONTROL, Id, /ENDEF

; Write proximity confidence
VarId = NCDF_VARID(Id, 'proximity_confidence')
NCDF_VARPUT, Id, VarId, proximity_confidence

; Write confidence flag
VarId = NCDF_VARID(Id, 'confidence_flag')
NCDF_VARPUT, Id, VarId, confidence_flag

; Write bias
VarId = NCDF_VARID(Id, 'SSES_bias_error')
index = where(SSES_bias_error ne -128.0, count)
if count[0] gt 0 then SSES_bias_error(index) = SSES_bias_error(index) / 0.01
SSES_bias_error = fix(SSES_bias_error)
NCDF_VARPUT, Id, VarId, SSES_bias_error

; write standard deviation
VarId = NCDF_VARID(Id, 'SSES_standard_deviation_error')
index = where(SSES_standard_deviation_error ne -128.0, count)
if count[0] gt 0 then SSES_standard_deviation_error(index) = SSES_standard_deviation_error(index) - 1.0
if count[0] gt 0 then SSES_standard_deviation_error(index) = SSES_standard_deviation_error(index) / 0.01
SSES_standard_deviation_error = fix(SSES_standard_deviation_error)
NCDF_VARPUT, Id, VarId, SSES_standard_deviation_error

; write dual nadir difference
VarId = NCDF_VARID(Id, 'atsr_dual_nadir_sst_difference')
index = where(diff ne -32768.0, count)
if count[0] gt 0 then diff[index] = diff[index] / 0.01
diff = fix(diff)
NCDF_VARPUT, Id, VarId, diff

;  Done
NCDF_CLOSE, Id

; Check all inputs/outputs are closed. Print end time to screen
close, /all
print, 'Finsished at: ', SYSTIME()


end
```