AATSR SST Retrieval:

Updated retrieval coefficients based on ARC project findings

Technical note for the ATSR QWG

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1 INTRODUCTION

The retrieval of Sea Surface Temperature (SST) from AATSR uses linear regression algorithms with coefficients derived from radiative transfer models (see for example Závody et al., 1995, Merchant et al., 1999) that perform a linear regression of SST to simulated brightness temperatures (BTs) at nominal band centres located at 3.7 µm, 11 µm and 12 µm, utilising either the nadir view or a combination of the nadir and forward view. Since launch, two different sets of retrieval coefficients have been used that are referred to as the *pre-launch* and *December 2005 Case 'C'* coefficients, respectively.

Each set can be identified according to their auxiliary filename:

- *Pre-launch*: ATS_SST_AXVIEC20020123_074408_20020101_000000_20200101_000000
- *December 2005 Case 'C'*: ATS_SST_AXVIEC20051205_102103_20020101_000000_20200101_000000

In addition, the *December 2005 Case 'C'* coefficients are supplemented by an additional latitude bias (Birks, 2006) to better align the dual 2-channel and dual 3-channel retrievals.

Various validation studies (O'Carroll et al., 2005, Corlett et al., 2006, Noyes et al., 2006, Barton 2006, Wimmer et al., 2010) have shown that:

- The dual 3-channel, dual 2-channel and nadir 3-channel retrievals have small but significant warm global biases compared to reference data (0.1 °C – 0.2 °C).
- The nadir 2-channel retrieval has a very large global bias compared to reference data (0.75 °C – 1.0 °C).
- The 2-channel retrievals have significant latitudinal variation in bias even after the latitudinal correction has been applied.
- All retrievals have a strong residual dependence on wind speed.
- All retrievals have regional variations in bias.

Significant improvements to all AATSR retrievals have been demonstrated as part of the ATSR Reprocessing for Climate (ARC) project (Embury et al., 2010). Although a lot of the improvement is due to the new formulation of the SST retrieval (in ARC the coefficients are banded by total column water vapour and not latitude), this report shows that the updated physical basis and forward modelling used in ARC provides improved SST retrievals compared to the current operational coefficients, even when banded by latitude.

2 PHYSICAL BASIS

The new coefficients are based on radiative transfer (brightness temperature simulation) selected at an early stage in the ARC project (Merchant et al., 2008). The basis in radiative transfer is fully described in a paper (Embury et al., submitted for Remote Sensing of Environment ATSR special issue), and is summarised in this section.

The simulation system (combination of radiative transfer models) comprises a gas transmittance model (that accesses a fundamental spectroscopic database and calculates transmittance through the atmosphere layer-by-layer and line-by-line), a surface spectral emissivity model (with inputs related to sea surface state), and a discrete ordinates solver that does the calculation of aerosol scattering and absorption.

The transmittance model is the Reference Forward Model (Dudhia, 2008) accessing v1.1 of the MT-CKD water vapour continuum model (Clough et al., 2005) and the HITRAN2000 (Rothman et al., 2003) spectroscopic database with updates to relevant species that were included later in HITRAN2004. “HITRAN2000 + updates” is consistent with the continuum parameterisation MT-CKD. The spectral resolution used was 0.01 cm^{-1}.

Seawater spectral emissivity is pre-calculated in look-up tables as a function of wind speed, viewing angle, wavelength, salinity and temperature, using an extension of previous approaches (Watts et al., 1996; Masuda, 2006) to include a synthesis of results for water refractive indices (including Newman et al., 2005).

The aerosol and scattering model exploits the solver DISORT, applied to channel integrated transmittances with and without aerosol to estimate the aerosol impact to be applied to the channel-integrated brightness temperatures without aerosol that come from RFM. The aerosol parameters are drawn from Optical Properties of Aerosols and Clouds (OPAC; Hess et al., 1998).

This simulation system is applied to selected atmospheric and surface states. The elements of defining these are:

- Radiatively active trace gas composition (assumed not to be variable with meteorology, but appropriate to the epoch for AATSR and covering seasonal climatological variations where important)
- Water and temperature profiles (a sample of meteorological conditions)
- Associated surface wind and temperature
- Aerosol profiles (marine and stratospheric-volcanic)

The meteorological states were defined as a subset of the representative ERA-40 selection of Chevallier (2002). Surface wind and temperature were from the matched surface fields, except for grid cells where a non-zero sea ice fraction means the skin temperature field partly reflects the ice surface temperature: in these cases an empirical model of a distribution representing SSTs near ice was randomly sampled.

Trace gases were included if they affect BT in any channel by 0.001 K or more. The trace gases simulated were: CO2, **O3**, **N20**, **CH4**, NH3, **HNO3**, OCS, *H2CO*, N2, ***C2H6***, **F11**, **F12**, *F22*, *F113*, *CCl4*, ***HNO4***. For those in bold, geographical and/or seasonal variations were important enough that these trace gas profiles were varied appropriately within the simulation set. Those in italic are additional compared to Zavody et al. (1995); their combined effect is ~40 mK in the 12 µm channel.

The mode of BT variability due to stratospheric-volcanic aerosols was calculated based on a Mie scattering model, indices of refraction for sulphuric acid, and observed size distributions following the Mt Pinatubo event.

Marine aerosols are included in the basic “clear sky” BTs on which coefficients are based, unlike stratospheric aerosols. An exponential decrease with height of number density of clean maritime aerosol particles is assumed, with OPAC surface concentrations and scale height on a 5 degree lat-lon grid. Anthropogenic and mineral aerosols are not included in the coefficient determination.

BT difference distributions based on the ARC simulation system were plotted following Merchant and Harris (1999), and compared with observed AATSR BT difference distribution and also with the legacy RAL-derived RTM used in Merchant and Harris (1999). In essence, the legacy RTM showed discrepancies in differences of order 0.2 to 0.4 K. With the new simulation system (having added 0.2 K to the suspect 12 µm channel – see below), they were mostly <0.1 K, and at worst 0.2 K for a limited range.

This basis in radiative transfer is identical to that specified in the Algorithm Theoretical Basis Document (ATBD) for the Sea and Land Surface Temperature Radiometer (SLSTR) SST.

3 COEFFICIENT GENERATION

The updated coefficients were generated as follows. BTs from the simulations described above for "clear sky" (but including marine aerosol) were regressed against the input SSTs used in the simulations for five channel combinations and for the nominal centre and edge of swath geometry assumed in the operational processing. This was done for the three latitude zones specified in Zavody et al (1995), which operational processing uses. The channel combinations are

- N2: nadir only, 11 and 12 µm
- N3: nadir only, 3.7, 11, and 12 µm
- D2: dual view, 11 and 12 µm
- D3: dual view, 3.7, 11, and 12 µm
- D2*: dual view, 3.7, 11

In the case of N2 and N3, the regression is unconstrained as in Zavody et al. (1995). In the case of D2, D3 and D2*, the regression is constrained such that coefficients are orthogonal to a mode of stratospheric-volcanic aerosol, using the equations in Merchant et al. (1999). The D2* retrieval was introduced within the ARC project to deal with the relatively large, not wholly explained, uncertainty in the 12 µm channel calibration for AATSR. It is used at locations of *in situ* observations where match-up data have been retained; all the above retrieval types are applied. Thus, the uncertainty in the 12 µm channel is bypassed in setting the overall bias of the retrievals in each latitude zone. It is implicitly assumed here that the variability of the 12 µm channel is affected only in second order by the calibration uncertainty and therefore the channel can still be used if its calibration offset is adjusted for in each latitude zone. Note that in simulation, D2* is as good a channel combination for retrieval as D3. The *in situ* data are not used at all in the definition of the offset adjustments.

Although the D2* approach is successful in ARC using a redesigned coefficient scheme, using latitudinal banded coefficients, all retrievals showed larger latitudinal variation in bias when compared to the D2* than for a global D3 retrieval. Consequently, all coefficients are averaged across each coefficient-latitude zone, and the N2, N3, D2 and D3 offset coefficients are adjusted to give the same mean SST as for global D3.

If no adjustment of 12 µm BTs is made, the adjustments made to the offset coefficients to bring them in line with global D3 are (for the high, mid and low latitude bands respectively in each case):

- N2: -0.28, -0.20, -0.02

- N3: -0.02, -0.04, -0.06
- D2: -0.17, 0.00, 0.12

If the 0.2 K is added to the 12 µm channel (as is done in ARC pre-processing, this being an approximate bias correction) then the offset coefficient adjustments are:

- N2: 0.16, 0.19, 0.24
- N3: 0.05, 0.08, 0.15
- D2: 0.10, 0.20, 0.27

The offset adjustments required are much more consistent between latitude bands when pre-adjustment of the 12 µm by 0.2 K is applied, suggesting the simulation system and that channel are in better agreement after adding 0.2 K to the channel.

Using the actual instrument radiometric noise will produce coefficients that are slightly less sensitive to radiometric noise, but at the cost of having larger systematic errors (see Embury et al., submitted to Remote Sensing of Environment ATSR Special Issue). Adding a small amount of noise is useful in conditioning the inversion that fixes the coefficients, and causes negligible bias. Therefore, a “noise” value of 0.01 K is included. The same coefficients should be used for both the 1-km and spatially averaged products.

4 ASSESSMENT METHODOLOGY

The assessment of the performance of the updated AATSR retrieval coefficients is through comparison to coincident drifting buoy observations. Existing match-up datasets (MD) used currently for AATSR validation were used. These are:

1. *The Met Office AATSR MD*
    - For assessment of spatially averaged 10' SSTs (ATS_AR__2P and ATS_MET_2P)
    - Includes a skin to drifter adjustment and diurnal flagging
    - Uses operational SADIST cloud screening
2. *The ARC AATSR MD*
    - For assessment of 1 km gridded SSTs (ATS_NR__2P)
    - Includes a skin to drifter depth adjustment and a diurnal warming adjustment
    - Forward view adjusted by -1 pixel along-track and -2 pixels across-track
    - 12 µm BTs adjusted by + 0.2 K
    - Uses Bayesian cloud screening

Further details on the Met Office AATSR MD can be found in O’Carroll et al. (2005) and details of the ARC MD can be found in Embury et al. (2010).

Six different set of coefficients were analysed. These are:

- **V0**: The current operational coefficients plus latitudinal correction of Birks (2006)
- **V1**: New coefficients, no latitude banding, no additional bias adjustment
- **V2**: New coefficients, latitude banding for all, no additional bias adjustment
- **V3**: New coefficients, latitude banding for all, adjusted to give ~ zero bias relative to global D3
- **V4**: New coefficients, latitude banding for N2, N3 and D2, global D3; all adjusted to give ~ zero bias relative to global D3
- **V5**: New coefficients, latitude banding for N2, N3 and D2, global D3; all adjusted to give ~ zero bias relative to global D3; +0.2 K added to all 12 micron BTs in retrieval.

V0 are the current operational coefficients and V4 are the updated coefficients proposed for implementation. V1, V2 and V3 are included for the interested reader to see the effect each refinement has on the residual bias when compared to drifting buoys. Results from comparing all five retrievals to drifting buoys using the Met Office MDB are provided in Section 5. In addition to the V0 to V4 comparisons, a further comparison (V5) was done to allow for a comparison between the 10' and 1 km results. For the 1-km results we have used the ARC MDB as this includes fields extracted from Level 1b products to allow reprocessing of SSTs. The ARC MDB makes allowance for several of the data quality issues currently affecting AATSR data. In particular, the forward view is adjusted by -1 pixel along-track and -2 pixels across-track, all 12 µm BTs are adjusted by + 0.2 K and it uses the Bayesian cloud screening. Consequently the results presented later in Section 5 for the 1-km product will benefit from allowing for these issues. It is expected that only the view-alignment will be fixed during the next processor upgrade so the updated SSTs will be degraded slightly due to the suspected 12 µm BT offset and the limitations of the operational SADIST cloud mask.

5 RESULTS

This section summarises the results from comparing AATSR SSTs retrieved using the updated retrieval coefficients to drifting buoys. Estimates of AATSR SST_{skin} for the both the 10' and 1 km product have been adjusted to estimates of $SST_{0.2\ m}$ using either the Saunders or Fairall plus Kantha-Clayson schemes. The actual depth of a drifting buoy measurement in the ocean is unknown so the sensor depth of 0.2 m is used as an approximation.

Figure 5-1 shows the updated ATS_AR__2P 10' $SST_{0.2\ m}$ minus drifting buoy SST as a function of latitude, wind speed and across-track pixel number. These results were generated from reprocessing the Met Office MDB using the various updated coefficients; the Met Office MD does not include an estimate of TCWV so this field remains blank in the plot. The right hand side of Figure 5-1 has results for the current operational coefficients (V0) and the left hand side shows results for the proposed new operational coefficients (V4).

For the latitudinal variation, little change is seen in the D3 retrieval although a reduction in residual bias across all latitudes is seen. Similar observations are true also for the N3 retrieval. Both the D3 and N3 retrievals are dominated by the strong linear dependency on TCWV at 3.7 µm, so little change would be expected for global coefficients stratified by latitude. Significant improvements are seen in both the D2 and N2 retrieval though. For the D2 retrieval, a lot of the residual latitudinal structure is removed and the updated D2 retrieval has very good agreement to the D3 between 50° S and 35° N, particularly at night; the large difference between the day time and night time D2 results is due to the Met Office MD only flagging diurnal heating event and not correcting for them. Remaining D2 biases for the new coefficients are of the order of 0.1 K. the largest improvement by far is for the N2 retrieval, which actually does not appear in the bias plots in Figure 5-1 as its current biases are so large. Unfortunately some residual bias will remain, although these are now much smaller than before and are of the order of 0.2 K, as a single view 2-channel retrieval coefficients banded by latitude are just not capable of retrieving sensibly under all atmospheric and surface conditions. Reducing the residual biases even more is possible by stratifying the retrieval coefficients by TCWV rather than latitude (Embury et al., 2010), however this would require a major change to the operational SST retrieval.

An improvement is seen in the wind speed dependency for the new coefficients, particularly for the nadir-only retrievals. The large residual day time biases are due to not adjusting for diurnal warming in the Met Office MD. The residual bias in the dual-view retrievals may be due to a remaining uncertainty in the forward view emissivity model, or it may be due to the current view alignment error, which is not corrected for in the Met Office MD, or could be due to residual cloud screening failures.

The new coefficients have improved the across track dependency for all retrievals, and the offset between the dual-view and nadir-only retrievals that is wind speed dependent is also apparent. Equivalent plots to Figure 5-1 for coefficients V1, V2, V3 and V5 are provided in Appendix 1 and the end of this document. Larger residual latitudinal variations are seen for both the day time D2 and N2 retrievals, which is most likely due to incorrect flagging of diurnal warming events in the Met Office MDB.

A summary of all match-up results using the Met Office MD is given in Table 5-1.

Retrieval/Version	N2	N3	D2	D3
V0 (Daytime)	+0.980 (0.44)		+0.225 (0.29)	
V0 (Nighttime)	+0.836 (0.45)	+0.072 (0.23)	+0.140 (0.29)	+0.145 (0.22)
V1 (Daytime)	+0.374 (0.43)		+0.196 (0.29)	
V1 (Nighttime)	+0.229 (0.44)	+0.032 (0.22)	+0.101 (0.29)	+0.054 (0.23)
V2 (Daytime)	+0.340 (0.40)		+0.220 (0.27)	
V2 (Nighttime)	+0.197 (0.40)	+0.015 (0.22)	+0.135 (0.27)	+0.079 (0.23)
V3 (Daytime)	+0.109 (0.39)		+0.128 (0.24)	
V3 (Nighttime)	-0.035 (0.40)	-0.015 (0.22)	+0.046 (0.25)	+0.059 (0.22)
V4 (Daytime)	+0.109 (0.39)		+0.128 (0.24)	
V4 (Nighttime)	-0.035 (0.40)	-0.015 (0.22)	+0.046 (0.25)	+0.054 (0.23)
V5 (Daytime)	+0.065 (0.39)		+0.086 (0.24)	
V5 (Nighttime)	-0.079 (0.40)	-0.046 (0.22)	+0.004 (0.25)	+0.022 (0.23)

Table 5-1: Summary of match-up results (median and robust standard deviation), in K, between AATSR 10' $SST_{0.2\ m}$ and drifting buoys. V0 are the current operational coefficients and V4 are the proposed new coefficients for implementation in the operational processor.

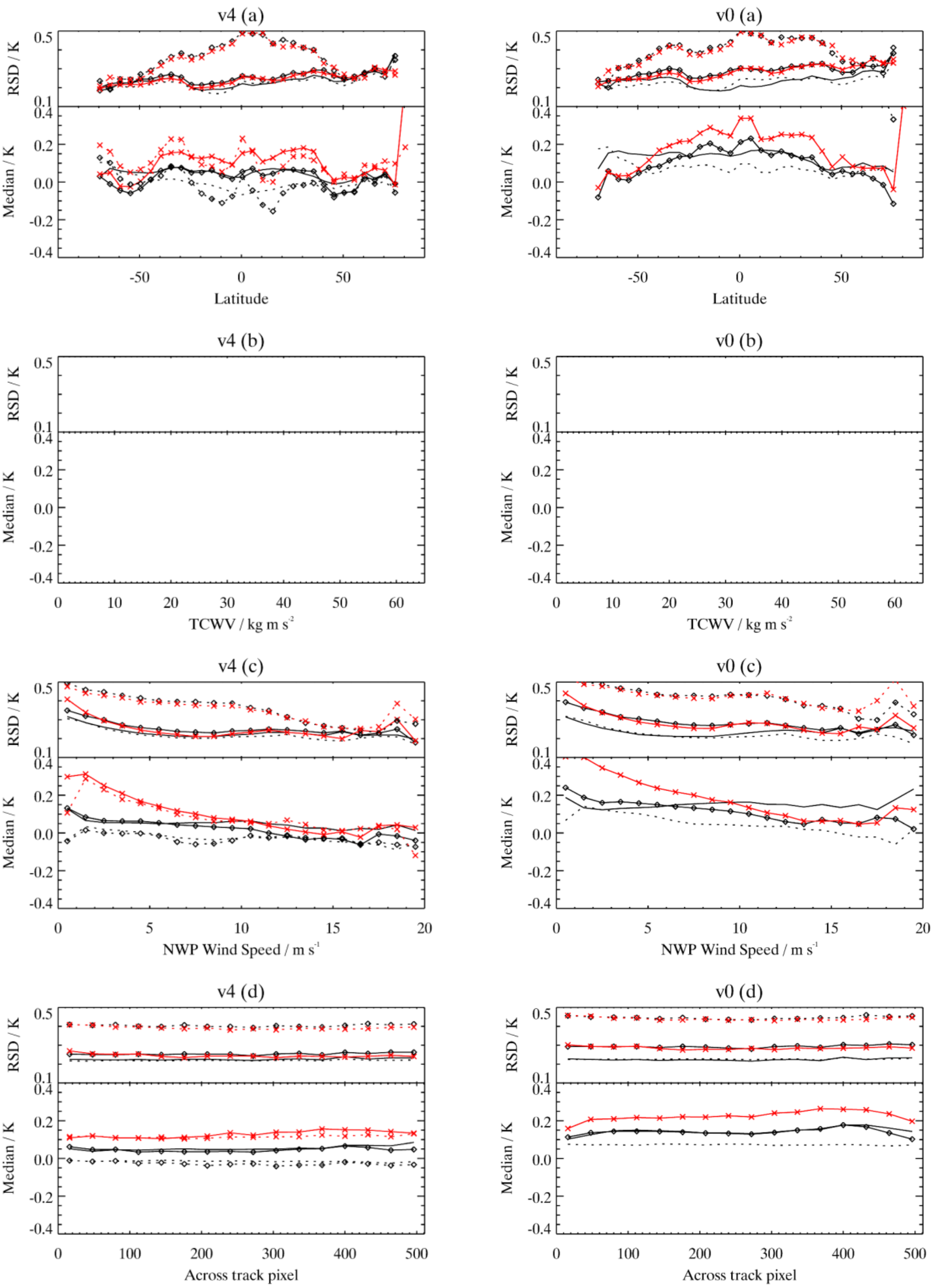

Figure 5-1: AATSR 10' estimated $SST_{0.2\ m}$ minus drifter SST as a function of latitude (a), TCWV (b), wind speed (c), and pixel position (d). Left column (V4) shows proposed new coefficients, right column (V0) shows current operational coefficients. Dashed with symbol = N2; dashed = N3; solid with symbol = D2; solid = D3. Black indicates night-time data; red (with x symbol) indicates day-time data. The Met Office MD does not include an estimate of TCWV so this field remains blank in the plot but is left in for ease of comparison with other figures.

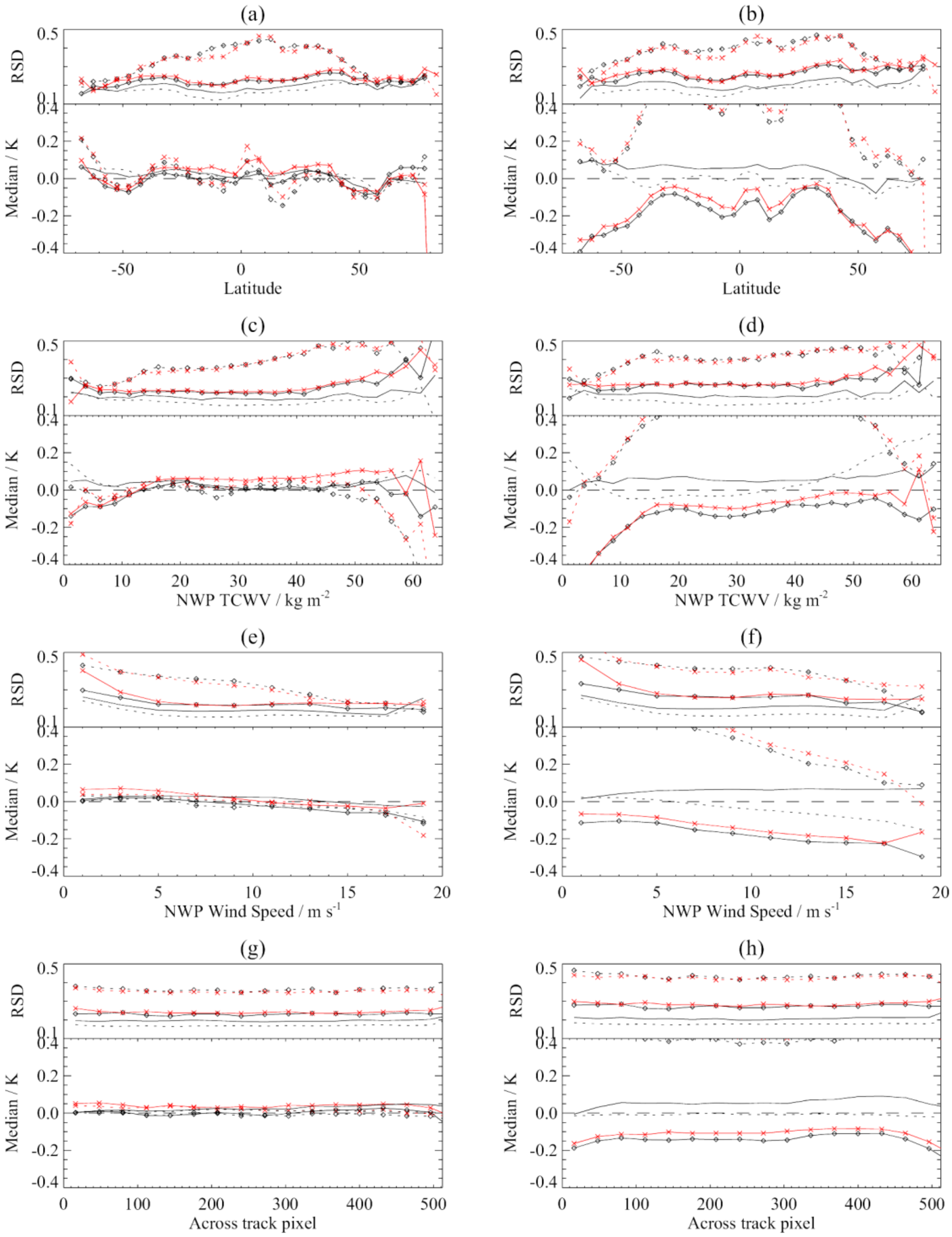

Figure 5-2: AATSR 1-km estimated $SST_{0.2\ m}$ minus drifter SST as a function of latitude (a, b), TCWV (c, d), wind speed (e, f), and pixel position (g, h). Left column (a, c, e, g) shows proposed new coefficients (V5), right column (b, d, f, h) shows ARC-modified current operational coefficients (V0). Dashed with symbol = N2; dashed = N3; solid with symbol = D2; solid = D3. Black indicates night-time data; red (with x symbol) indicates day-time data.

Figure 5-2 shows the updated ATS_NR__2P 1-km $SST_{0.2\ m}$ minus drifting buoy SST as a function of latitude, TCWV, wind speed and across-track pixel number. The right hand side of Figure 5-2 has results for the ARC-modified current operational coefficients and the left hand side shows results for the proposed new coefficients. The findings are very similar to those for the 10' results, allowing for the ARC-modifications (addition of + 0.2 K to all 12 µm BTs and adjustment of forward-view to better align with nadir-view) and we see much better agreement between day time and night time D2 and day time and night time N2 results as the ARC MDB uses a diurnal warming model to adjust the SSTs rather than simply flag expected cases of diurnal warming. Some of the improvement will also be due to the use of the Bayesian cloud screening as well as allowance for the suspected 12 µm offset. Indeed, the effect of the 12 µm offset can be seen in Table 5-1 where adding + 0.2 K in the V5 results causes a 0.03 K shift compared to V4. The N2/N3/D2 coefficients are of course adjusted to have near-zero bias relative to the global D3 coefficients, so they've all picked up the same 0.03 K (+/- the fitting error) shift.

A summary of all match-up results using the ARC MD is given in Table 5-2.

Retrieval/Version	N2	N3	D2	D3
V0 (Daytime)	-0.157 (0.37)		-0.099 (0.26)	
V0 (Nighttime)	-0.182 (0.38)	-0.059 (0.17)	-0.135 (0.24)	0.027 (0.20)
V5 (Daytime)	+0.020 (0.35)		+0.039 (0.24)	
V5 (Nighttime)	-0.007 (0.36)	0.012 (0.17)	+0.004 (0.23)	0.025 (0.20

Table 5-2: Summary of match-up results (median and robust standard deviation), in K, between AATSR 1 km $SST_{0.2\ m}$ and drifting buoys. V0 are ARC-modified operational retrievals and V5 are the proposed new coefficients for implementation in the operational processor but include the ARC corrections for the 12 µm BTs and the view-alignment.

6 SUMMARY

This report summarises the generation and assessment of new retrieval coefficients for AATSR. The new coefficients have been generated using updated physical basis developed as part of the ARC project. We recommend the updated coefficients (V4, latitude banding for N2, N3 and D2, global D3; all adjusted to give ~ zero bias relative to global D3) are implemented operationally for AATSR.

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8 APPENDIX 1

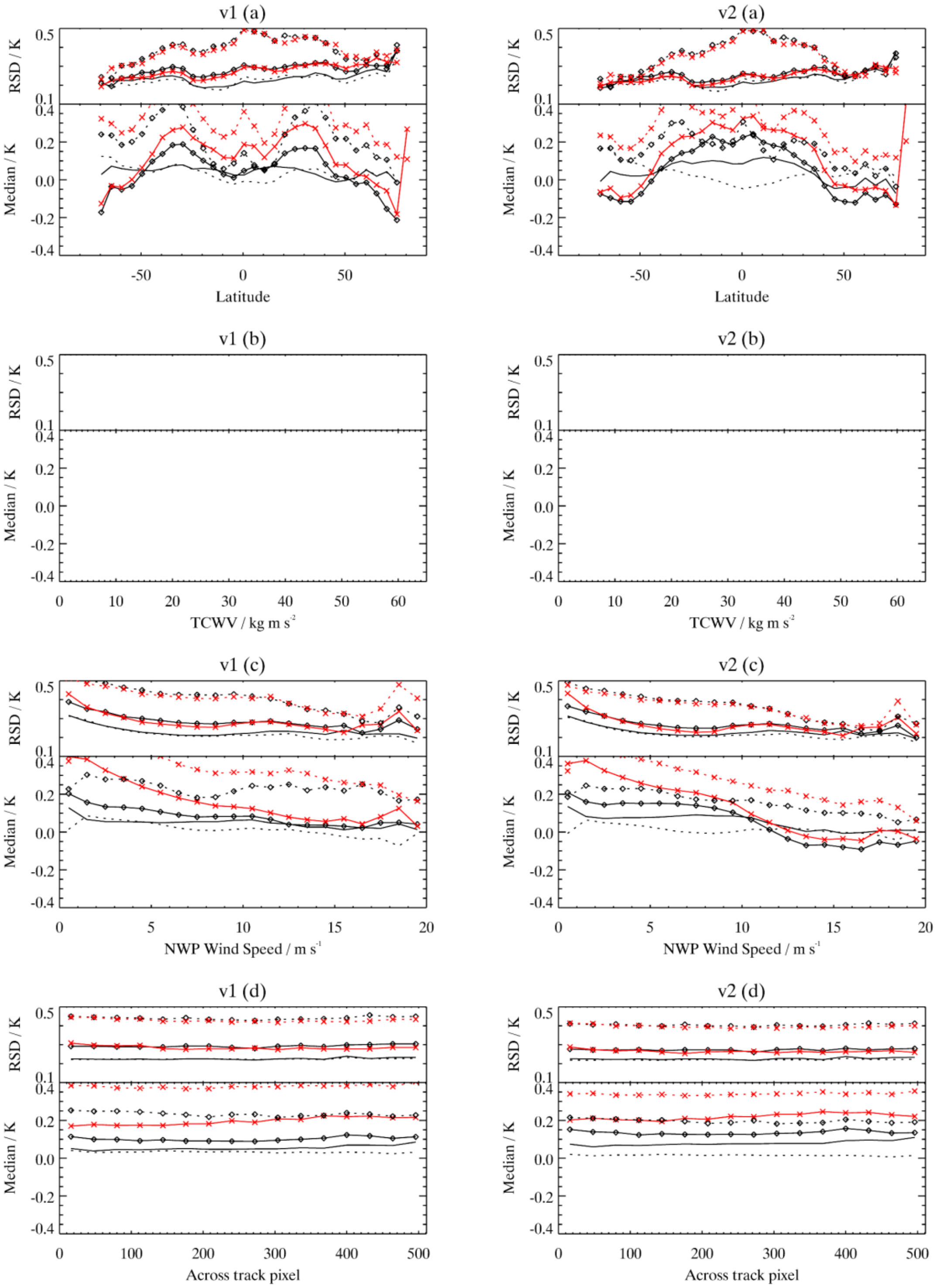

Figure 8-1: As per Figure 5-1 but for V1 (left hand side) and V2 coefficients (right hand side).

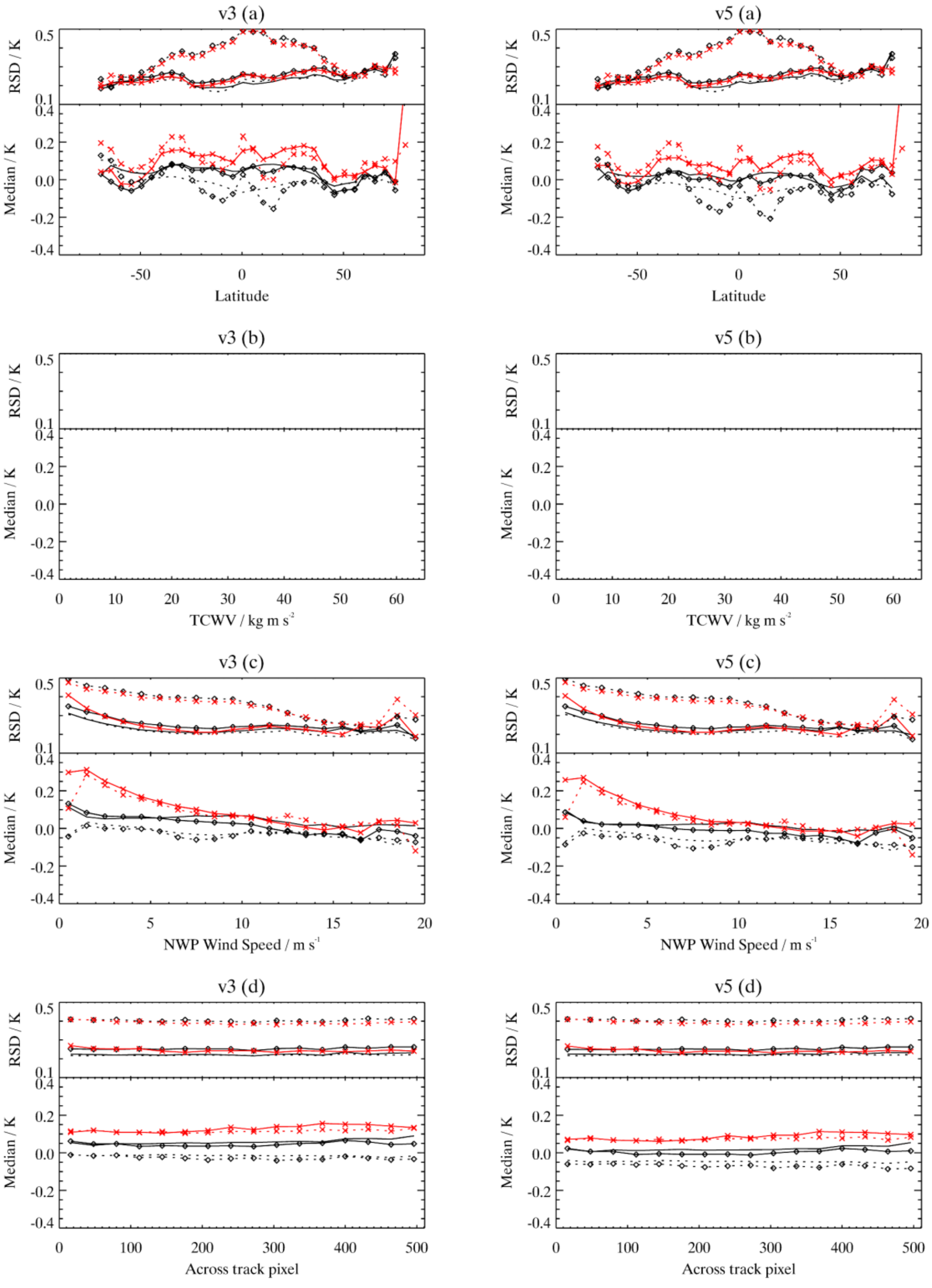

Figure 8-2: As per Figure 5-1 but for V3 (left hand side) and V5 coefficients (right hand side).