National Weather Service
National Centers for Environmental Prediction

Technical Procedures Bulletin

Series No: MMAB/2006-01

Subject: The daily Real-Time, Global Sea Surface Temperature – High Resolution Analysis: RTG_SST_HR

January 5, 2006 MMAB, Environmental Modeling Center, Camp Springs, MD 20746-4304

THIS TPB WILL SUPERCEDE TPB 477 ON THIS PRODUCT IN DECEMBER 2006

This bulletin, prepared by Mr. William Gemmill, Mr. Bert Katz, Dr. Xu Li, and Mr. Lawrence Burroughs for the National Centers for Environmental Prediction (NCEP), Environmental Modeling Center (EMC), describes upgrades to the daily real-time, global sea surface temperature analysis (RTG_SST), which was originally implemented on 30 January 2001. See TPB 477 for a description of that analysis. The new analysis with the upgrades is designated as RTG_SST_HR and was implemented into operations September 27, 2005. The original RTG_SST will continue to run in parallel for 6-12 months to allow for comparisons by users. These products are used by NCEP's regional North American Model (NAM) and ECMWF's global forecast model as ocean surface boundary conditions, and also by researchers studying air-sea interactions. Each daily product uses the most recent 24-hours of *in situ* and satellite-derived surface temperature data and provides a global SST on a 1/12 ^{o} x 1/12 ^{o} longitude/latitude grid. As part of the analysis system, there is a separate evaluation program that runs following the analysis.

The daily Real-Time, Global Sea Surface Temperature – High Resolution Analysis: RTG_SST_HR[1]

by

William Gemmill[2]
Bert Katz[3]
Xu Li[4]
Lawrence D. Burroughs[2]

1. Introduction

The original daily Real-time Global Sea Surface Temperature analysis (RTG_SST) was implemented on January 30, 2001 (See TPB 477 and Thiebaux *et al* 2003). The analysis has run reliably over the past four years, and is used by the regional North American Model (NAM; Black 1994) at the National Centers for Environmental Prediction (NCEP) and by the global forecast model at the European Center for Medium Weather Forecasting (ECMWF). This analysis has been used for various marine applications, *i.e*. Chelton & Wentz (2005) have used it to describe air-sea interactions for regions that contain strong SST fronts. But the RTG_SST analysis has limitations, because of its resolution (1/2 degree), in resolving the temperature structure of ocean features, coastal zones and bays and inland lakes. The NCEP's Global Forecast System (GFS) still uses the Reynolds-Smith SST (1994). Tests of the GFS using the RTG_SST showed that its forecast skill was slightly degraded, when compared to the GFS using the Reynolds-Smith SST. It was found that the RTG_SST day to day difference fields are noisy (as much as 0.5ºC–1.0ºC) which is likely due to the accuracy and distribution of the various data sets. See figure 1 for a review of some of the limitations of the RTG_SST analysis.

1) Does not resolve meso-scale features well (*i.e.,* Gulf Stream, Eddies, *etc.*)
2) Does not resolve inland lakes well or not at all.
3) Has large day to day temperature differences (sometimes as large as 0.5ºC – 1.0ºC), which are associated with the operational satellite retrievals provided by the Shared Processing Center.

Figure 1. Limitations of the RTG_SST analysis.

As a result of the RTG_SST day to day noise, an alternative SST retrieval method was developed at NCEP through collaboration with the Joint Center for Satellite Data Assimilation (JCSDA). This SST retrieval algorithm is based on variational principles (physical algorithm) which determines the SST increment to the SST first guess of the control variables using the previous day's SST analysis, GFS model air temperature and GFS model (appendix 1). A cost function is defined to include (1) the analyzed control variables and their first guess differences and (2) observed AVHRR radiances and the analyzed radiances (using a radiative transfer model). See figure 2 for a review of the JCSDA retrieval method. These retrievals show improvements over the current "operational" retrievals processed by the U. S. Navy and received at NCEP from the SST Shared Processing Center (SPC) at the Naval Oceanographic Office (May *et al*, 1998). Those SST's are based on

[1] MMAB Contribution Number: 249
[2] EMC, MMAB
[3] SAIC
[4] JCSDA

1) Developed as alternative SST retrieval method
   a) Based on a physical retrieval (variational) algorithm which runs within the structure of the GDAS (Derber and Xu Li).
   b) Cost function minimizes the increment between;
      i) Observed radiances and simulated radiances, and
      ii) Analyzed SST and its first guess
2) Requires radiative transfer model to simulate Brightness Temperatures for each channel using
   a) SST first guess (previous analysis)
   b) Air Temperature (GDAS analysis)
   c) Water vapor mixing ratio (GDAS analysis)

Figure 2. Outline of JCSDA retrieval method.

regression equations which relate brightness temperature to SST values by using drifting buoys (McClain *et al* 1985, Walton *et al* 1997).

The new high resolution (RTG_SST_HR) analysis was implemented September 27, 2005 for operational use at NCEP. The RTG_SST_HR runs on a 1/12 degree grid, by using *in situ* data and physical retrievals from both NOAA-16 and NOAA-17 satellite data. The analysis package was upgraded to execute efficiently on multiple processors, rather than on one processor as in the original. The upgrade uses an MPI anisotropic recursive filter code (Purser *et al*, 2003) taken from the NCEP Grid-point Statistical Interpolation (GSI) analysis (Treadon *et al*, 2005). Table 1 presents a comparison of the original SST analysis system with the upgraded system.

Table 1. A summary of the of the original and new daily SST analysis systems.

	RTG_SST	**RTG_SST_HR**
Horizontal resolution	½ Degree latitude/longitude grid	1/12 Degree latitude/longitude grid
***In situ* Data**	Fixed buoys, drifting buoys & ships	Fixed buoys, drifting buoys & ships
Satellite Data	NOAA 16 AVHRR	NOAA 16 & 17 AVHRR
Satellite Processing	Navy – Regression Retrievals	JCSDA – Physical Retrievals
Analysis computation time	1 processor – 0.3 min	20 processors - 3.5min
AVHRR Limitations	Can not see through clouds	Can not see through clouds

In summary the major upgrades are:

1) Increased grid resolution to 1/12 degree,
2) Data from two satellites – NOAA 16 and 17, and
3) SST generated by the JCSDA physical retrieval system.

2. Description of RTG_SST_HR

The original RTG_SST code (summarized in figure 3) was modified and adapted to run on the IBM-SP computer. The new real-time global high-resolution sea surface temperature analysis is produced daily on a $1/12^{o}$ x $1/12^{o}$ lon/lat grid.

The algorithm (Parrish 2004) starts with a first-guess analysis, which is the previous day's SST analysis with a one day climate adjustment. *In-situ* observations for the last 24-h and high-resolution (4 km) satellite retrievals are ingested next. The SST data from moored buoys are averaged over the 24-h period; while SST reports from ships and drifting buoys are averaged separately within each $1/12^{o}$ x $1/12^{o}$ grid box over the last 24-h. The satellite SST retrievals are generated within NCEP by using the JCSDA physical retrieval algorithm (See appendix by Li). Biases in the retrievals are removed by using an analysis of the previous 7 days of *in situ* data only. For each grid box, four averages are made from the satellite retrievals: a day and night average for each satellite (NOAA 16 and 17). Where the satellite observed ice cover exceeds 50 percent a SST is computed by taking the Levitus (1982) salinity climatology into account and following Millero's (1978) formula. The analysis error correlation function is given by Cor = $\exp(-d^2/\ell^2)$, where d is the distance between data and analysis grid-point locations, and ℓ the analysis error length scale. Both d and ℓ are in km. The length scale error varies from 100 to 450 km depending on the climatological temperature gradient. It is determined from ℓ = min(450, max(225/|gradT|, 100)), where gradT is the climatological temperature gradient. ℓ is on the order of 100 km in high gradient areas (Gulf Stream or Kuroshio) and on the order of 450 km in small gradient areas (Sargasso Sea).

Following the completion of the analysis, a separate verification program is run, which is described in section 3.

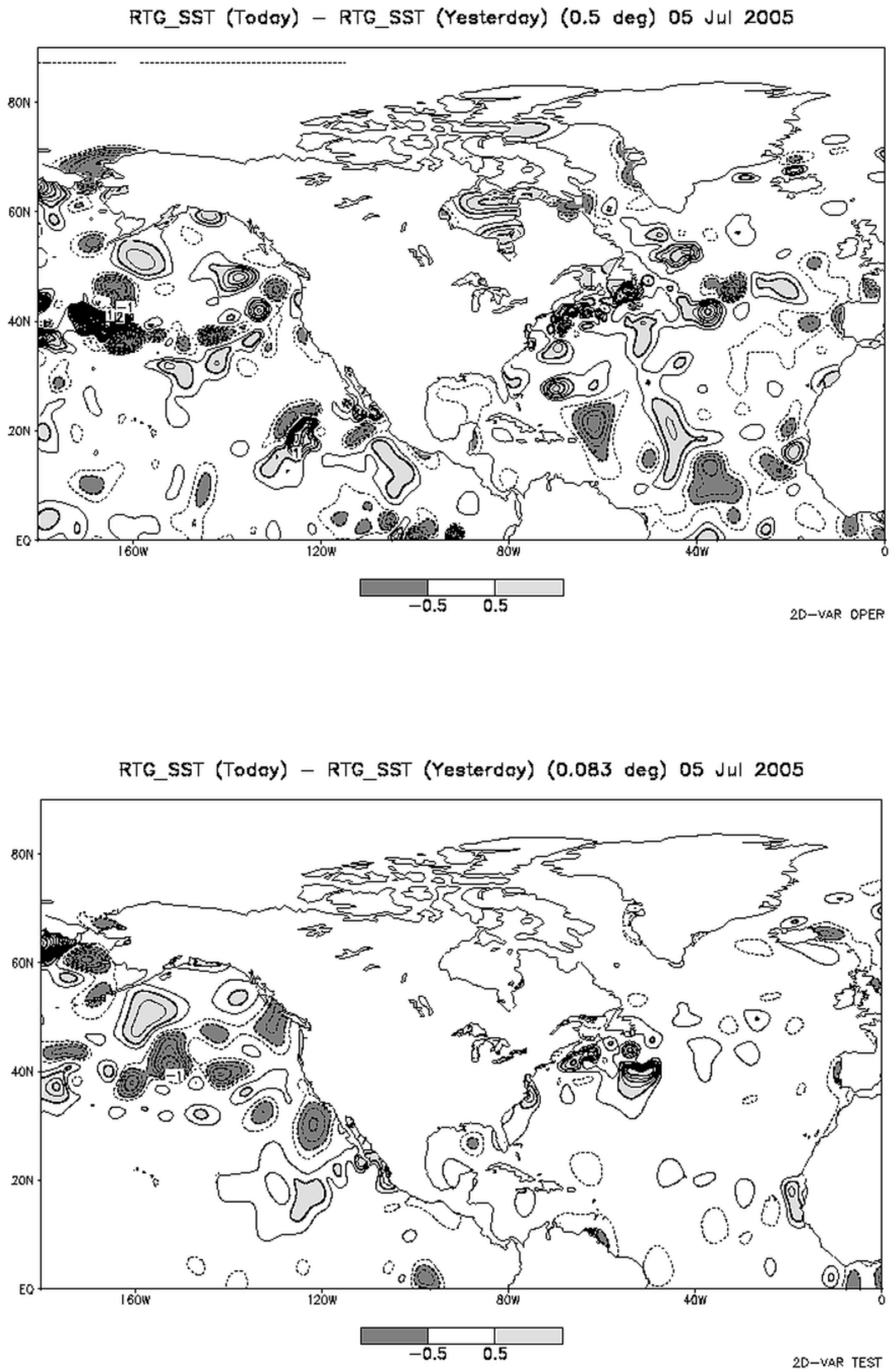
3. Evaluation of the RTG_SST_HR

The new RTG_SST_HR has been evaluated by comparing it with the RTG_SST. Since one of the problems of the RTG_SST was the day to day noise, the first concern was to compare the day to day SST changes for each of the analyses (figures 3). The physical retrievals reduced the day to day SST changes "noise", especially in the tropics. Further, the impact of satellite retrievals, regression, produced by the Shared Processing Center (SPC), or physical, produced by the JCSDA, on its SST analysis shows that the physical retrievals also reduces the satellite retrieval biases.

An evaluation of the satellite SST retrievals with drifting buoy data is shown in Table 2. This table shows that the accuracy of the physical SST retrievals is improved over those from the SPC. Further, the night time retrievals are better than the day time retrievals. That is due to the day time contamination by sun glint near 3.7μm (channel 3) of the AVHRR instrument.

Table 2. Summary of the evaluation of SST retrievals from SPC and JCSDA for satellites NOAA 16 & 17 using AVHRR data and separated for day and night using drifting buoys as ground truth.

Satellite	Time	Mean Error	RMS Error
Shared Processing Center (regression retrievals)			
NOAA 16	Day	0.02	0.56
	Night	-0.01	0.44
NOAA 17	Day	0.09	0.39
	Night	-0.02	0.35
Joint Center for Satellite Data Assimilation (physical retrievals)			
NOAA 16	Day	0.03	0.43
	Night	-0.08	0.39
NOAA 17	Day	-0.04	0.35
	Night	-0.04	0.32



(a)

(b)

Figure 3. Comparison of day-to-day noise levels (a) RTG_SST; (b) RTG_SST_HR. Note that (b) has less day-to-day noise than (a).

An evaluation of the satellite SST retrievals with drifting buoy data is shown in Table 3. In reality, the statistics are even over the globe, but the RTG_SST_HR are slightly worse over the North West Atlantic (Gulf Stream). It is suspected that the correlation length scales need to be tuned for coastal regions and mesoscale ocean features (Gulf Stream).

Table 3. Summary of the evaluation of the two analysis systems for global and a selected region for the mean bias, and mean RMS using drifting buoys as ground truth.

Global	Operational (1/2D)	-0.02	0.53
	JCSDA Retrievals (1/12D)	0.01	0.51
Gulf Stream	Operational (1/2D)	-0.07	0.90
	JCSDA Retrievals (1/12D)	0.02	0.96

An internal verification program is executed for both versions of the SST analysis following the conclusion of the analysis itself. The verification statistics are generated by rerunning the analysis programs five times, each time withholding an independent subset of the pre-selected buoys (about 20%), and evaluating the resulting analysis at the locations of the withheld data. The bias and root-mean-square (RMS) difference between the independent buoys and the analysis are computed for each subset. Global statistics can be difficult to interpret since many parts of the world's ocean are homogeneous and differences are small.

4. Further Tuning for RTG_SST_HR Analysis

In developing the new SST analysis, the number of upgrades to the original SST system was kept to a minimum. This was done in order to make interpretation relatively straight forward and to implement it into operations as soon as possible. The physical SST retrievals reduce the day to day noise in the analysis and the satellite bias, but the statistics comparing the two analysis show little difference between them.

The following is a short list of items which will be tested to determine what impact they have on improving the analysis:

1) Correlation length scales for the 1/12 degree grid,
2) Error assignments for each SST data set and the background field,
3) An-isotropic correlation length scales, which are important along zones of large SST gradients and along coast lines, and a
4) New high resolution climatology.

5. References

Black, T. L. (1994): The New NMC mesoscale Eta model: Description and forecast examples. *Wea. Forecasting*, **9**, 265-278.

Chelton, Dudley B., and Frank J. Wentz (2005): Global Microwave Satellite Observations of Sea-Surface Temperature for Numerical Weather Prediction and Climate Research, *Bull. AMS*, **86**, 1097-1115.

Levitus, S. (1982): Climatological atlas of the world. *NOAA Professional Paper 13*, 173 pp.

May, Douglas A, Michelle M. Parmeter, Daniel S. Olszeski, and Bruce D. McKenzie (1998): Operational Processing of Satellite Sea Surface Temperature Retrievals at the Naval oceanographic Office, *Bull. AMS*, **79**, 397-407.

McClain, E. P., W. G. Pichel and C. C. Walton (1985): Comparative performance of AVHRR-based multichannel sea surface temperatures *Geophysical Research*, **90**, 587-11,601.

Millero, F.J., (1978): Freezing point of seawater. Eighth Report of the Joint Panel on Oceanographic Tables and Standards, *UNESCO Tech. Pap . Mar. Sci.* No. 28, Annex **6**, UNESCO, Paris.

Parrish, DF (2004): Personnel communications.

Purser, R.J., W.S. Wu, D.F. Parrish and N.M. Roberts, (2003): Numerical aspects of the application of recursive filters to variational statistical analysis; Part II: Spatially inhomogeneous and anisotropic general covariances. *Mon Wea Rev*, **191**, 1536-1548

Reynolds, Richard, W. and Thomas M. Smith (1994): Improved Global Sea Surface Temperature Analyses Using Optimum Interpolation, *J of Climate*, 929-948.

Thiebaux J, Eric Rogers, Wanqiu Wang and Bert Katz (2003): A New High-resolution Global Sea Surface Temperature Analysis, *Bull. AMS*, **84**, 645-656.

Treadon, Russell, (2005): First GSI User Orientation, 4-5 Jan 2005, WWB, Camp Springs, MD. [http://www.emc.ncep.noaa.gov/gbm/treadon/gsi/]

Walton, CC, WG Pichel, and JF Sapper (1998): The Development and Operational application of Nonlinear algorithms for the Measurement of Sea Surface Temperatures with the NOAA Polar-orbiting Environmental Satellites, *J. Geophys. Res.*, **103**, c12, 27999-28012.

Appendix 1

Sea Surface Temperature (SST) Physical Retrieval Algorithm

Xu Li

A.1. Formulation

The basic principle of the physical (or variational) SST retrieval algorithm is to find out the increment to the first guess of the control variables, which may contribute to the radiative transfer, by minimizing a cost function which measures the distances between (1) The analyzed control variable and its first guess and (2) observed radiance and the analyzed (modeled) radiance

.

Generally, the variational assimilation or retrieval problem is to minimize the following cost function:

$$J = J_b + J_o = \underbrace{\frac{1}{2}(X^a - X^f)^T B^{-1}(X^a - X^f)}_{(1)} + \underbrace{\frac{1}{2}[y - H(X^a)]^T O^{-1}[y - H(X^a)]}_{(2)} \qquad \text{(a1.1)}$$

Here, ^{a},^{o} ,^{f} represents analysis, observation and first guess respectively. X is the vector of control variables, y is the observation vector. B , O is the error covariance matrix of the X^f and y respectively. H is the .observation operator, which can be the interpolation operator or radiative transfer model. ^{T} means transpose.

A radiative transfer model is required to simulate the first guess radiance and written as:

$$T_{b,c}^f = H_c[T_s^f, T_k^f, Q_k^f] \qquad \text{(a1.2)}$$

Here, T_k^f and Q_k^f is the first guess (6-hour forecast) of the atmospheric temperature and water vapor mixing ratio, respectively, for model layer $k = 1, L$.

T_s^f is the first guess of the SST retrieval (previous SST analysis here). c is the satellite instrument (AVHRR) channel index. $T_{b,c}$ is the brightness temperature of channel c .

Generally, for channel c , the analysis increment of T_b from T_b^f can be written as:

$$\delta T_{b,c} = T_{b,c}^a - T_{b,c}^f = \frac{\partial T_{b,c}}{\partial T_s} \cdot \delta T_s + \sum_{k=1}^{L}\left(\frac{\partial T_{b,c}}{\partial T_k} \cdot \delta T_k\right) + \sum_{k=1}^{L}\left(\frac{\partial T_{b,c}}{\partial Q_k} \cdot \delta Q_k\right), \text{ where} \qquad \text{(a1.3)}$$

$$\delta T_s = T_s^a - T_s^f, \delta T_k = T_k^a - T_k^f, \delta Q_k = Q_k^a - Q_k^f .$$

The derivatives $\frac{\partial T_{b,c}}{\partial T_s}$, $\frac{\partial T_{b,c}}{\partial T_k}$ and $\frac{\partial T_{b,c}}{\partial Q_k}$ are available from the radiative transfer model and represent the sensitivity of the radiances to the analysis variables. To simplify the problem, it is assumed that δT_k and δQ_k are not dependent on altitude (k) and are written as δT_a and δQ_a , respectively, this gives:

$$\delta T_{b,c} = T_{b,c}^a - T_{b,c}^f = \frac{\partial T_{b,c}}{\partial T_s} \cdot \delta T_s + \frac{\partial T_{b,c}}{\partial T_a} \cdot \delta T_a + \frac{\partial T_{b,c}}{\partial Q_a} \cdot \delta Q_a, \text{ where} \qquad \text{(a1.4)}$$

$$\frac{\partial T_{b,c}}{\partial T_a} = \sum_{k=1}^{L} \frac{\partial T_{b,c}}{\partial T_k}, \quad \frac{\partial T_{b,c}}{\partial Q_a} = \sum_{k=1}^{L} \frac{\partial T_{b,c}}{\partial Q_k} .$$

Therefore, T_s, T_a and Q_a become the control variables of the variational retrieval problem. There are no explicit expressions for T_a^f, Q_a^f. However δT_a, δQ_a share the increments caused by the difference between the observed ($T_{b,c}^a$) and simulated ($T_{b,c}^f$) radiances in the retrieval process. This is required to account for the attenuation of the radiances by atmosphere.

Let $\sigma_s, \sigma_a, \sigma_q$ be the error of T_s, T_a and Q_a. Let $\sigma_{b,c}$ be the error of the simulated radiance for channel c. The retrieval is done for each datum, the errors of first guess and observation are assumed to be uncorrelated. Therefore,

$$X = \begin{pmatrix} T_s \\ T_a \\ Q_a \end{pmatrix}, \ y = \begin{pmatrix} T_{b,3} \\ T_{b,4} \\ T_{b,5} \end{pmatrix}, \ B = \begin{pmatrix} \sigma_s^2 & 0 & 0 \\ 0 & \sigma_a^2 & 0 \\ 0 & 0 & \sigma_q^2 \end{pmatrix}, O = \begin{pmatrix} \sigma_{b,3}^2 & 0 & 0 \\ 0 & \sigma_{b,4}^2 & 0 \\ 0 & 0 & \sigma_{b,5}^2 \end{pmatrix}$$

Where X represents variables of X^a and X^f

Therefore, the cost function becomes

$$J = \frac{1}{2\sigma_s^2}(\delta T_s)^2 + \frac{1}{2\sigma_a^2}(\delta T_a)^2 + \frac{1}{2\sigma_q^2}(\delta Q_a)^2 + \frac{1}{2}\sum_c \frac{1}{\sigma_{b,c}^2}[T_{b,c}^o - (T_{b,c}^f + \delta T_{b,c})]^2 \tag{a1.5}$$

$J = J_{\min}$ when $\frac{\partial J}{\partial T_s} = \frac{\partial J}{\partial T_a} = \frac{\partial J}{\partial Q_a} = 0$, this gives three linear equations with three unknowns:

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} \delta T_s \\ \delta T_a \\ \delta Q_a \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} \tag{a1.6}$$

Let $w_s = \frac{1}{\sigma_s^2}, w_a = \frac{1}{\sigma_a^2}, w_q = \frac{1}{\sigma_q^2}$, $w_c = \frac{1}{\sigma_{b,c}}, S_c = \frac{\partial T_{b,c}}{\partial T_s}, A_c = \frac{\partial T_{b,c}}{\partial T_a}, Q_c = \frac{\partial T_{b,c}}{\partial Q_a}, T_c = T_{b,c}^o - T_{b,c}^f$ for AVHRR nighttime retrievals with channel $c = 3, 4, 5$,then

$$a_{11} = w_s + w_3 S_3^2 + w_4 S_4^2 + w_5 S_5^2,$$
$$a_{22} = w_a + w_3 A_3^2 + w_4 A_4^2 + w_5 A_5^2,$$
$$a_{33} = w_q + w_3 Q_3^2 + w_4 Q_4^2 + w_5 Q_5^2$$

$$a_{12} = a_{21} = w_3 S_3 A_3 + w_4 S_4 A_4 + w_5 S_5 A_5,$$
$$a_{23} = a_{32} = w_3 A_3 Q_3 + w_4 A_4 Q_4 + w_5 A_5 Q_5$$
$$a_{31} = a_{13} = w_3 S_3 Q_3 + w_4 S_4 Q_4 + w_5 S_5 Q_5$$

$$c_1 = w_3 S_3 T_3 + w_4 S_4 T_4 + w_5 S_5 T_5,$$
$$c_2 = w_3 A_3 T_3 + w_4 A_4 T_4 + w_5 A_5 T_5,$$
$$c_3 = w_3 Q_3 T_3 + w_4 Q_4 T_4 + w_5 Q_5 T$$

The solution of (a1.5) gives three increments; only δT_s is used to obtain the SST retrieval.
The errors used in the retrieval scheme are as follows:

1) Day-time, $\sigma_s = 0.5, \sigma_a = 1.2, \sigma_q = 0.95 \times \{\max[(T_s^f - 273.16) \times 0.03, 0.0]\}$

2) Night-time, $\sigma_s = 0.45, \sigma_a = 0.9, \sigma_q = 0.65 \times \{\max[(T_s^f - 273.16) \times 0.03, 0.0]\}$

3) NOAA-16, $\sigma_{b,3} = 0.12, \sigma_{b,4} = 0.16, \sigma_{b,5} = 0.18$;

4) NOAA-17, $\sigma_{b,3} = 0.11, \sigma_{b,4} = 0.17, \sigma_{b,5} = 0.19$.

A.2 AVHRR Radiance Bias Correction

A bias correction is applied to the AVHRR radiance dynamically based on 2-week observed and simulated radiances with a look-up table in which the correction amount depends on the SST value.

A.3 Quality Control

Initially if the difference between the observed and the modeled radiance exceeds a threshold value for a given channel, the radiance datum is discarded and not used. The threshold of rejection is given by:

$$abs(T_{b,c}^o - T_{b,c}^f) > 10.0 \times \sigma_{b,c}.$$