Implementation of Version 6 AQUA and TERRA SST processing

K. Kilpatrick , G. Podesta, S. Walsh, R. Evans, P. Minnett
University of Miami
March 2014

<u>Outline of V6 MODIS SST changes</u>:

- A total of 3 additional correction terms were added to both the LWIR SST and MWIR SST4 algorithm formulations; 2 terms are related to a satellite zenith angle correction and a single term relating to a mirror side correction
- Coefficients were estimated and are applied by latitude band and month of generic year.
    - The LWIR SST algorithm no longer selects coefficients based on brightness temperature difference as a proxy for water vapor.
- Changes to SST Flag thresholds
    - SSTREFDIFF changed to a cold only tests SST – REFSST >= -3.0 to prevent flagging, as bad, good pixels which may be warmer than reference as a result of the diurnal heating of the skin surface at low wind speeds during the day.
    - SSTREFDIFF modified to include a more stringent cold threshold (SST – REFSST) >= -1.25, in regions likely to be contaminated by dust where retrievals are generally colder. Dust Region is defined as falling within a latitude <= 30N and > 10S and longitude of and between 105 E and 105W.
    - SSTF CLOUD binary decision trees added to identify pixels with contaminated atmospheres (dust absorbing aerosols ect) not captured by uniformity tests.
- Quality level definition changes
    - Quality 0 and Quality 1 definitions differ only by the SST Flag HISENZ and BTNONUNIF flag.
    - Quality level of daytime pixels in glint regions, that are otherwise clear in all SST flags, can be no better than 1 due to visible band tests not being valid in the glint region
    - Quality levels of pixels with the BTVNONUNIF set is changed to be no better than 3.
    - Quality level of pixels with the SSTF CLOUD flag set can be no better than a 3. An inherited coding error was found in the version V5 code at OBPG, and traced to the original MODAPS code, whereby the SST CLOUD bit was being set but not evaluated in regard to the final quality level.
    - Pixels failing the SSTREFDIFF are now assigned to Quality level 2
    - Quality level 3 and better will be binned in global maps, previously only quality 2's and better were included.

Overview

Aggregate global comparisons of night time MODIS version 5 sea surface skin temperatures to *in situ* buoy observations, for the life of each mission through 2013, indicate that the long wave infrared (LWIR) skin SST from TERRA and AQUA respectively, have biases of -0.145 and -0.250 and standard deviations of 0.510 and 0.509, relative to the subsurface temperatures measured by the global network of drifting buoys. Mid-wave Infrared (MWIR) SST4 product biases for TERRA and AQUA are -0.095, and -0.180 with standard deviations of 0.422 and 0.423. These aggregated statistics for V5 are quite good for both sensors for pixels assigned the best quality level, ql=0, and are close to the expected theoretical pseudo sub-surface skin difference of -0.17 (Kearns et. al. 2000 ; Donolon 2002). The standard deviations of ~0.5 is similar to heritage sensors. Detailed times series, regional analysis, and global comparisons to other products such as Reynolds and microwave derived SST products indicate three systematic patterns in residuals that will be reduced or eliminated in the version 6 reprocessing. In version 6 changes were made in regard to how correction factors for response versus scan angle (RVS) and mirror side are determined and subsequently applied, and algorithm coefficients are latitude based. When these changes are combined with minor adjustments to quality level definitions and thresholds for some SST flags, the uncertainty is decreased by ~0.1 and seasonal regional biases are reduced.

Methods and motivation for changes

MODIS SST Version 5 trends include an asymmetric variation across the scan (figure 1) and differences between mirrors (figure 2) that remained even after the previously implemented SST specific corrections for RVS and mirror side had been applied during processing.

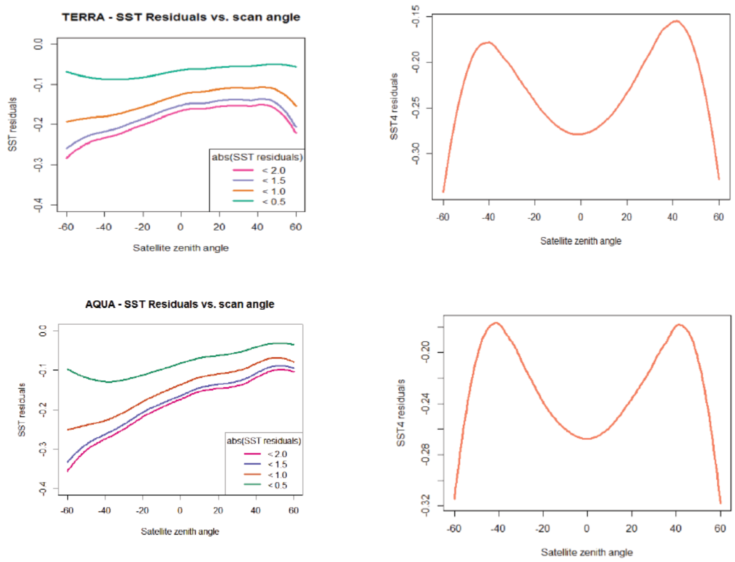

Figure 2: Linear fit of residual RVS as a function of satellite zenith angle. LWIR panels left panels at different magnitudes of residuals. MWIR panels right panels for TERRA and AQUA respectively. A trend in the central tendency of both Terra and AQUA SST residuals is clearly apparent. For the LWIR SST on Terra, a pattern of increasing residuals from -60° to 0° satellite zenith angle (SZA) is observable with a plateau from 0 to 50°and followed by a parabolic roll off. On Aqua, the trend is more linear across the entire scan -60° to 60°.

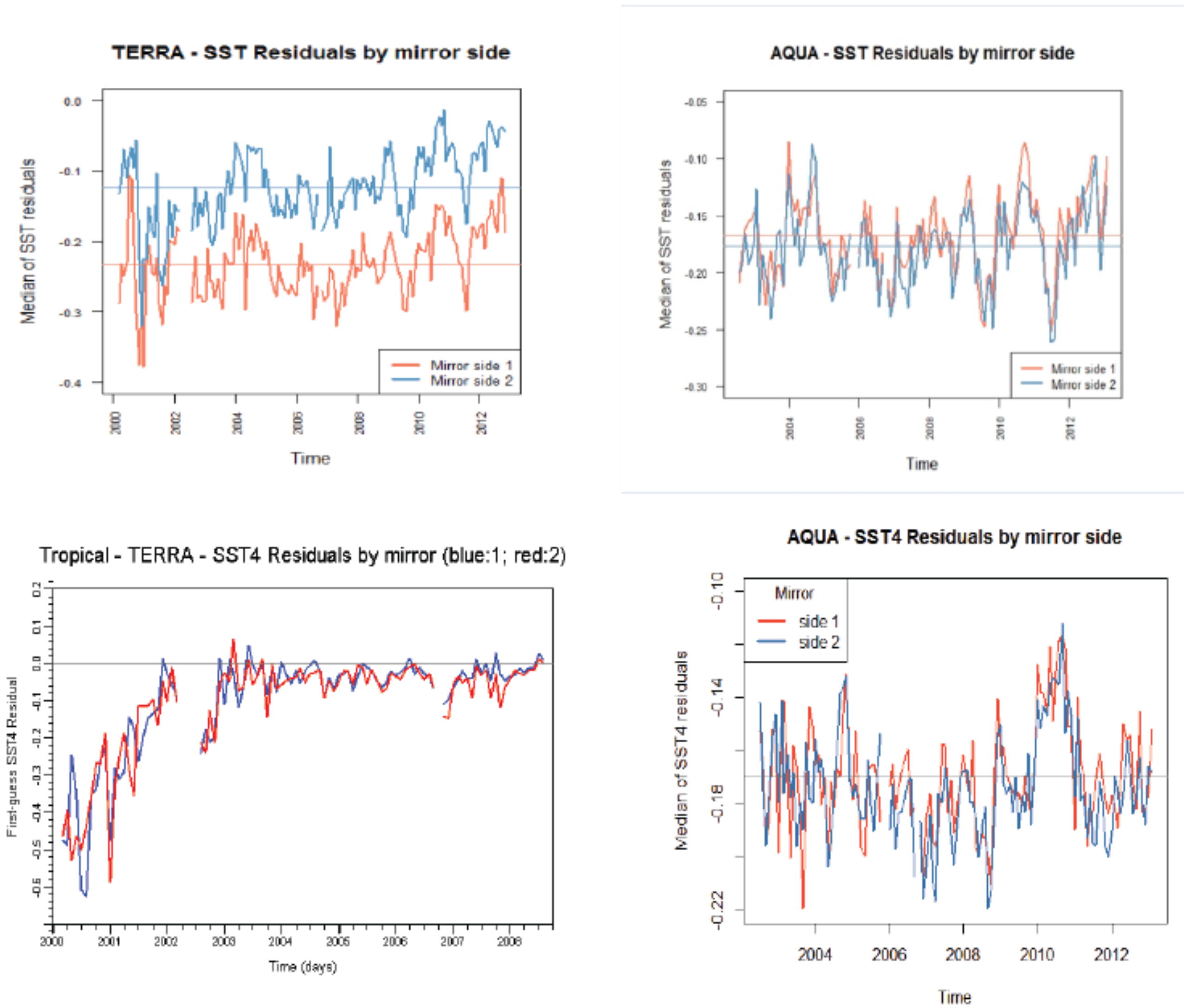

Figure 2: Times series of median residuals SST and SST4 residuals by mirror side. Left : TERRA right :AQUA Top: LWIR; bottom: MWIR. Note: scale difference between plots.

In addition to the RVS and mirror difference, some regions exhibit strong seasonal differences as a function of latitude (figure 3) particularly near the poles, despite the use of time and water vapor dependent coefficients.

Figure 3. Time Series plot of error characteristics for version 5 and version 6 relative to *in situ* buoys for each latitude band. Both sensors V5 (red) show varying degrees of repeating seasonal trends in different latitude bands, particularly at the poles. These trends are reduced in Version 6 (blue).

To reduce the RVS and mirror side artifacts three new terms were added to the base algorithm formulation. These terms correspond to a single term to capture changing mirror side differences, and two terms to capture both the linear and second-degree quadratic shape of differences in retrievals across satellite zenith angle. The previous corrections developed for V5 had been made in "SST space", and applied as ad hoc corrections after the SST was calculated. The motivation for adding additional correction terms to the algorithm form was to allow a more robust empirical approach to the corrections in brightness temperature space and better capture any changes in the amount of correction as a smooth function of viewing geometry, surface temperature, time and latitude.

The "updated" forms of the algorithms are:

$SST_{sat} = a_0 + a_1 BT31 + a_2(BT31-BT32)\ T_{sfc} + a_3(\sec(\theta)-1)(BT31-BT32)) + a_4(mirror.side) + a_5(\theta) + a_6(\theta)^2$

$SST4\ sat = a_0 + a_1 BT22 + a_2(BT22-BT23) + a_3(\sec(\theta)-1) + a_4(mirror.side) + a_5(\theta) + a_6(s\theta)^2$

In version 6 coefficients are estimated as a function of both month of year and latitude band, rather than the traditional 5 month sliding window for high and low water vapor regimes. The goal of latitude based month of year coefficients is to reduce the residual seasonal effects in each hemisphere seen in V5, which we believe is due in part to the global distribution of buoys, used for coefficient estimation, being dominated by buoys located in the mid-latitudes of the Northern hemisphere. Empirical coefficients from these buoys do not always reflect the conditions at other latitudes, particularly in Polar Regions where the emissivity of the cold surface and a dry atmosphere can be very different.

The coefficient estimations were made using a generalized linear model, run multiple times to create 72 sets of coefficients corresponding to 12 months times six latitude bands. All terms in this formulation may not necessarily be significant in all of the 72 sets, and a term's significance may be unique to either AQUA or TERRA. To obtain the most parsimonious model, for each month and latitude band, the Akaike Information Criterion (AIC) was used to compare models. In sets where terms in the full model were not significant, coefficients for these non-significant terms are set to zero and the reduce model is used.

Quality level and flags changes

Quality level definitions were modified slightly with six goals .

- The first goal was to make the definitions more uniform, between both day and night and across missions. That is, combinations of SSTFLAGS used to define a specific quality level are more similar between day and night and between missions.
- The second goal was to improve the uncertainty characteristics of pixels at higher scan angles by requiring pixels assigned to quality level 1 to have the

same combination of SST flags clear as quality 0, except scan angles are greater than 55 or uniformity is <= 1.2.

- ❖ The third goal was to prevent daytime pixels that were warmer than the reference, due to diurnal warming of the sea surface skin at low wind speeds, from being assigned a poor quality. To accomplish this the SSTREF test was changed to be a cold only test during the daytime.
- ❖ The fourth goal was to prevent pixels contaminated by dust, which are just slightly cold, from being assigned to the quality 0 population. The SSTREF flag threshold was modified to be more stringent, >= -1.25, in regions likely to be contaminated by dust defined as within the box latitude <= 30N and > 10S and longitude of and between 105 E and 105W. This reduces the cold bias occasionally seen in the global images off of Africa, regions of the Mediterranean, and Indian ocean during dust events.
- ❖ The fifth goal was to indicate that daytime pixels contaminated by glint may have higher uncertainty because thresholds for the visible band cloud tests are not valid in glint regions, decreasing the ability to identify clouds. Pixels in glint regions can be assigned no better than quality 1.
- ❖ The sixth goal was to prevent pixels at frontal edges that had previously been assigned to the worst quality, due to failing SSTREF test in high gradient regions, from being masked in global images as the worst quality and not binned. The pixels at frontal edges that fail the SST reference test but are not truly bad are now assigned to quality level 2.

OBPG SST Web page quality/flag tables updated for Version 6

V6 Quality Tests

A series of quality tests are performed for each sst or sst4 retrieval. The quality tests are used to set the quality levels, which are then used to control the Level-3 binning process. For the msl12 implementation, each quality test was assigned a bit in a product-specific flag array. A separate, 16-bit flag product was created for both the short-wave (sst4) and long-wave (sst) products (flags_sst4 and flags_sst, respectively). The 16 flag bits were assigned as follows:

Bit	Name	Description
00	ISMASKED	Pixel was already masked
01	BTBAD	Brightness temperatures are bad
02	BTRANGE	Brightness temperatures are out-of-range

03	BTDIFF	Brightness temperatures are too different
04	SSTRANGE	SST outside valid range
05	SSTREFDIFF	SST is too different from reference
06	SST4DIFF	Longwave SST is different from shortwave SST
07	SST4VDIFF	Longwave SST is very different from shortwave SST
08	BTNONUNIF	Brightness temperatures are spatially non-uniform
09	BTVNONUNIF	Brightness temperatures are very spatially non-uniform
10	BT4REFDIFF	Brightness temperatures differ from reference
11	REDNONUNIF	Red-band spatial non-uniformity or saturation
12	HISENZ	Sensor zenith angle high
13	VHISENZ	Sensor zenith angle very high
14	SSTREFVDIFF	SST is too different from reference
15	CLOUD	Pixel failed the cloud decision tree

- ISMASKED Set if the SST processing is not performed because the pixel was masked prior to invocation. The msl12 code allows the user to specify a number of masking conditions. For standard SST processing, the only condition which would likely be selected for masking by msl12 at this stage is if the pixel is over land.

- BTBAD Set if the observed radiances are beyond the limits of the radiance to brightness temperature tables, such that brightness temperatures can not be determined. This generally indicates saturation of one of the critical IR channels.

- BTRANGE Set if one of the brightness temperatures falls outside the physically realistic range for ocean observations. The currently accepted range for all IR bands except for the 4um channel is -4 to 37 deg-C. The 4um band has a range of -4 to 35 deg-C.

- BTDIFF Set if the brightness temperature difference falls outside the physically realistic range for ocean observations. For long-wave SST, dBT = BT11 - BT12 and the currently accepted range for dBT is 0 to 3.6 K. For short-wave SST, dBT = BT39 - BT40 and the currently accepted range for dBT is 0 to 8 K.

• SSTRANGE Set if the SST retrieval falls outside the physically realistic range for ocean observations. The currently accepted range is -2 to 40 deg-C during the day and -2 to 37 degrees night.

• SSTREFDIFF Set for the area outside a box defined a latitude <= 30N and > 10S and longitude of and between 105 E and 105W if during the night the absolute difference between the SST retrieval and the sstref (oisst) value exceeds 3 K and in the Daytime if the difference is colder only than - 3 K. Inside the box, difference is a more stringent cold threshold (SST – REFSST) >= -1.25K. The difference test may be problematic in regions of high spatial variability (e.g., frontal boundaries), as the sstref field is very low in spatial resolution and smoothed over time.

• SST4DIFF This test is only applicable at night. Set if the absolute difference between the long-wave and short-wave SST retrieval exceeds 0.8 K.

• SST4VDIFF This test is only applicable at night. Set if the absolute difference between the long-wave and short-wave SST retrieval exceeds 1.0 K.

• BTNONUNIF Set if one of the required brightness temperatures shows evidence of spatial non-uniformity. The uniformity is determined by examination of the 3x3 pixel area around the pixel of interest. If the difference between the maximum value and the minimum value in that 9-pixel set exceeds 0.7 K, the bit is set. This test does have a tendency to flag frontal boundaries and coastlines, as can be seen in this animation.

• BTVNONUNIF Set if one of the required brightness temperatures shows a high degree of spatial non-uniformity. The test is identical to that of BTNONUNIF, but with a larger threshold. If the difference between the maximum value and the minimum value in the 9-pixel set exceeds 1.2 K, the bit is set.

• BT4REFDIFF This test is only valid at night. The test compares the brightness temperature difference (dBT=BT39-BT40) against a supplied reference temperature, where the reference is provided as a function of scan pixel and accounts for the non-water vapor atmospheric absorption between the channels, e.g. ozone, etc. A plot of the dBTref is shown **here**. If the difference between dBT and dBTref falls outside a specified range, the bit is set. The currently acceptable range is -1.1 to 10.0 K.

• REDNONUNIF This test is only valid for daytime, and therefore only relevant to the long-wave SST product. Top-of-atmosphere reflectance (rho_t) in the 678-nm band (MODIS band 14) is computed over the 3x3 pixel area centered on the pixel of interest, where rho_t = pi*Lt/F0/(mu0 t t0 toz) and Lt is observed TOA radiance, F0 is band-averaged solar irradiance (at day of year), mu0 is cosine of solar zenith angle, t0 and t are the diffuse transmittance through a Rayleigh atmosphere (solar path and sensor path), and toz is the ozone transmittance (inbound and outband). If the difference between the maximum value and the minimum value of rho_t in the 9-pixel set exceeds 0.01, the bit is set.

This bit is also set if 8 or more of the 9 pixels are saturated in the 678-nm band. In general, such saturation might indicate the presence of clouds, but it may also indicate the presence of sun glint. The long-wave SST is affected by clouds (SST retrieval appears colder than normal), but not by sun glint. To recover the sun glint case, the REDNONUNIF bit is only set if the retrieved SST is more than 1 deg-C colder than the reference. This secondary requirement works best in locations with temporally and spatially stable SST conditions, where the low-resolution sstref and the retrieved SST can be expected to be consistent. The saturation test is a much more stringent test than the original uniformity test. The new test can be summarized as: set if red band reflectance in the pixel neighborhood is (saturated OR spatially nonuniform) AND SST retrieval is cold relative to the reference.

- HISENZ Set if the sensor zenith angle exceeds 55 degrees. For msl12, this is redundant with the HISATZEN bit in the l2_flag array, but with a different standard threshold.

- VHISENZ Set if the sensor zenith angle exceeds 75 degrees. This is rare.

- SSTREFVDIFF Set to indicate that the difference between the retrieved SST and the reference is very large (5-deg K). The related flag, SSTREFDIFF, indicates that the difference between the retrieved SST and the reference is moderately large (3-deg C).

- SST_CLOUD Set if pixels fail either the day or night decision tree indicating a likely problem/contaminate in the atmosphere that may lead to failure of the SST atmospheric correction algorithm. Note:the SST_cloud flag is not the same as the OC_cloud flag.

Quality Levels

The quality tests described above are used to set quality levels between 0 and 4, where 0 indicates best quality and 4 indicates complete failure or masked (usually land). The quality level determination varies between day and night conditions, and between the short-wave and long-wave SST products. The following tables show the quality test bits and associated quality levels. If no bits are set then the quality level is 0, but for short-wave SST retrievals in daylight the quality level is always set to 3 (bad) or 4 (failed or not computed). The quality level information for each SST product, sst and sst4, can be output by msl12 as products qual_sst and qual_sst4, respectively.

Daytime Long-Wave SST

Quality Bit	Minimum Quality Level
ISMASKED	4
BTBAD	4
VHISENZ	3
BTRANGE	3
SSTRANGE	3
BTVNONUNIF	3
SSTREFVDIFF	3
CLOUD	3
REDNONUNIF	2
SSTREFDIFF	2
BTNONUNIF	1
GLINT	1
HISENZ	1
	0

During the daytime if the SST-reference < -1 K and red band reflectance is high, rhot > 0.05 (where rhot is pi*Lt/F_0), the pixel quality is demoted one level.

Nighttime Long-Wave SST

Quality Bit	Minimum Quality Level
ISMASKED	4
BTBAD	4
BTRANGE	3
SSTRANGE	3
BT4REFDIFF	3
SSTREFVDIFF	3
CLOUD	3
BTVNONUNIF	3
VHISENZ	3
SST4VDIFF	2
SSTREFDIFF	2
BTNONUNIF	1
SST4DIFF	1
HISENZ	1
	0

At night the SST quality is demoted one level if the shortwave BTNONUNIF is set

Daytime Short-Wave SST

Quality Bit	Minimum Quality Level
ISMASKED	4
BTBAD	4
	3

Nighttime Short-Wave SST

Quality Bit	Minimum Quality Level
ISMASKED	4
BTBAD	4
BTRANGE	3
SSTRANGE	3
BT4REFDIFF	3
CLOUD	3
BTVNONUNIF	3
VHISENZ	3
SSTREFVDIFF	2
SST4VDIFF	2
SSTREFDIFF	1
BTNONUNIF	1
SST4DIFF	1
HISENZ	1
	0

Level-2 Flags

The Level-2 products produced by msl12 include a standard set of flags associated with each pixel, stored in the l2_flags SDS. Most of these flags have no explicit meaning for SST, as they were designed to work in the reflected solar regime. This includes the cloud flag. The bits of interest for SST are the SSTFAIL and SSTWARN. In previous versions of msl12, SSTFAIL was set when long-wave SST could not be calculated, and SSTWARN was set when long-wave SST was very different from the reference SST (Reynolds). These bits will now be set based on the SST quality levels described above. The SSTWARN or SSTFAIL bits in l2_flags will only be set if one or both of the SST products (sst or sst4) is requested for output to the Level-2 file.

Level-2 Flags

Bit	Name	Description
27	SSTWARN	SST quality is reduced
28	SSTFAIL	SST quality is bad

- SSTFAIL If the sst (or sst4) product is requested for output, this bit will be set in l2_flags if qual_sst (or qual_sst4) is greater than or equal to 4.
- SSTWARN If the sst (or sst4) product is requested for output, this bit will be set in l2_flags if qual_sst (or qual_sst4) is greater than or equal to 1.