REDESIGNED SINGLE SENSOR ERROR STATISTICS IN THE ADVANCED CLEAR-SKY PROCESSOR FOR OCEANS

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ABSTRACT

A redesigned algorithm for estimation of Single Sensor Error Statistics (SSES) for the baseline regression SST (BSST) product of the NOAA Advanced Clear-Sky Processor for Oceans (ACSPO) is described. The algorithm employs segmentation of the SST domain in the space of regressors (i.e., terms of the regression equation). For each segment, local regression coefficients and SDs are estimated from the corresponding subsets of matchups with quality controlled *in situ* data. SSES bias is estimated as the difference between the BSST and an auxiliary Piecewise Regression (PWR) SST produced with the local coefficients. Subtracting SSES biases from BSST reduces the effects of residual cloud, angular dependence of biases and, during the daytime, diurnal surface warming. This results in a significant reduction in global SDs of fitting *in situ* SST bringing them close to a level typical for “foundation L4” minus *in situ* SST statistics. While the CMC L4 SST is typically colder than daytime *in situ* SST, the PWR SST is consistent with *in situ* data during both day and night. The PWR SST may thus be viewed as an estimate of the “depth” SST and can potentially be a better input for assimilation into L4 SST systems, aimed at producing the foundation SST.

1. Introduction

The GHRSST Data Specification format (GDS 2.0) requires that Single Sensor Error Statistics (SSES), i.e. estimates of bias and standard deviation (SD) of retrieved SST, should be appended to each pixel of an L2/L3 SST product. Currently different processing centers employ different SSES definitions. The GHRSST-XV meeting has reviewed existing SSES practices and suggested revisiting those (Proceedings of GHRSST-XV, 2014). In particular, it was noted that no available SSES improves assimilation of L2 or L3 products into the existing L4 analyses. In this context, the initial SSES implementation (Petrenko and Ignatov, 2014b) used in the earlier versions of the NOAA Advanced Clear-Sky Processor for Oceans (ACSPO) SST retrieval system, has been redesigned with the explicit objective to provide a measurable improvement for L4 analyses. Customarily, assimilation of L2 or L3 product into L4 analyses is preceded by a “bias correction” in satellite SSTs with respect to *in situ* SSTs (or with respect to some reference satellite product). Therefore in the new SSES development, the primary objective was to significantly reduce biases in ACSPO SST relative to *in situ* SSTs. Moreover, the SSES SDs should provide a realistic measure of SST uncertainty in pixel, to allow optimization of L2/L3 SST weights during their assimilation into L4. Only the performance of SSES bias correction has been explored so far and it is documented in this paper. The new SSES was implemented in ACSPO v2.40 which became operational at NOAA on 19 May 2015.

2. Methodology

As documented in Petrenko et al. (2014a), the baseline SSTs (BSST, T_S) are produced in ACSPO with the regression equations proposed by Lavanant et al. (2012). Each equation is used with a single set of regression coefficients trained on a global dataset of matchups (MDS). Errors of fitting *in situ* SST with BSST are largely caused by inaccuracy of approximation of a highly variable inverse relationship between BTs and SST with one global regression equation and with a single set of coefficients. As a result, BSST errors essentially depend on observational conditions, i.e. on such variables as view zenith angle (VZA), total precipitable water vapor content in the atmosphere (TPW), etc.

To properly account for the above dependencies, SSES should be separately estimated for different segments of the SST domain relatively uniform in terms of retrieval errors. The previous ACSPO SSES algorithm stratified the SST domain by VZA and TPW. That approach, however, was found inefficient because the real number of physical variables affecting the retrieval errors is not limited by VZA and TPW. In fact, it is not obvious if it is possible at all to account for all physical factors essentially affecting retrieval errors (including, e.g., underscreened clouds), even with increased number of physical variables.

Instead, the redesigned ACSPO SSES considers the retrieval errors as functions of regressors (i.e. the terms on the right-hand side of the regression equation, excluding the offset), rather than certain geophysical variables. This limits the number of the SSES arguments, no matter how many physical variables the regressors depend on. The criteria for segmentation of the SST domain in the space of regressors (**R**-space) are derived from the statistics of regressors within the training MDS. Once such criteria have been established, the SST pixels and matchups are ascribed to specific segments based on the regressors' values. SSES SDs are estimated for each segment from the corresponding subset of matchups with quality controlled *in situ* data from *i*Quam (Xu and Ignatov, 2014). Note that we use a combination of drifters and tropical moorings in ACSPO Cal/Val analyses including the SSES. These subsets of matchups are also used to calculate local regression coefficients specific to each segment. The SSES SDs and local regression coefficients for all segments are stored in the lookup table (LUT). During the L2 production, the SSES SDs for every SST pixel are obtained from the LUT and the SSES biases are calculated as differences between the BSST and a Piecewise Regression SST (the PWR SST) calculated with the local regression coefficients.

3. Evaluation of SSES bias correction

As mentioned above, in the redesigned ACSPO SSES, the bias is defined as difference between BSST and PWR SST. Accordingly, applying SSES biases to the BSST transforms it into the PWR SST. Table 1 compares global statistics of fitting *in situ* SSTs in the matchups with BSST and PWR SST over the global MDS collected from 15 May 2013 to 8 August 2014 for VIIRS (onboard S-NPP), MODIS (onboard Aqua and Terra), AVHRR FRAC (on Metop-A and -B) and AVHRR GAC (on NOAA-19). The statistics of fitting *in situ* SSTs in the matchups with the L4 SST by the Canadian Met Center (CMC, Brasnett, 2008) are also shown. Since the data shown in Table 1 used the same MDS for both training and validation, the global biases for both algorithms are 0. PWR SST substantially reduces global SDs compared to BSST. Since CMC is constructed from nighttime satellite retrievals and *in situ* SSTs, it is biased cold with respect to daytime matchups, more so for the afternoon platforms S-NPP, Aqua and NOAA-19. The PWR SSTs do not show daytime biases typical for CMC but bring the global SDs closer to (or even smaller than) the corresponding SDs for CMC minus *in situ* SSTs. Further analyses based on subdividing the MDS into different time intervals and using one of them for training the coefficients, and another one for validation the derived SSTs have demonstrated the temporal stability of the BSST and PWR SST statistics with respect to *in situ* SST.

Table 1. Global biases and SDs of fitting *in situ* SST with BSST, PWR SST and CMC over the full MDS collected from 15 May 2013 – 8 August 2014.

SST	Statistics	S-NPP VIIRS	Aqua MODIS	Terra MODIS	MetOp-A AVHRR	MetOp-B AVHRR	NOAA19 AVHRR
				Day			
BSST	Bias	0	0	0	0	0	0
	SD	0.41	0.45	0.46	0.48	0.49	0.50
PWR SST	Bias	0	0	0	0	0	0
	SD	0.31	0.33	0.32	0.33	0.33	0.34
CMC	Bias	-0.19	-0.20	-0.06	-0.02	-0.03	-0.21
	SD	0.34	0.34	0.31	0.31	0.31	0.35
				Night			
BSST	Bias	0	0	0	0	0	0
	SD	0.33	0.35	0.35	0.46	0.45	0.46
PWR SST	Bias	0	0	0	0	0	0
	SD	0.25	0.26	0.26	0.30	0.30	0.29
CMC	Bias	0.01	0.02	-0.04	-0.08	-0.07	0.03
	SD	0.27	0.28	0.29	0.31	0.31	0.29

The redesigned SSES methodology was implemented in ACSPO v2.40 (with both L2P and L3U products) and used for processing some test data from six satellite sensors listed above. Fig. 1 demonstrates the effects of daytime and nighttime SSES bias correction by showing the geographical distributions of deviations of BSST and PWR SST from CMC for the S-NPP VIIRS L2P product on 16 February 2015, and corresponding SSES biases. The daytime deviations of BSST from CMC are mainly caused by cloud leakages, daytime warming in the upper surface layer of the ocean and variations in VZA. Nighttime SSES biases are also dependent on VZA and cloud leakages. SSES biases reflect all these effects, to a various degree. This makes correction of SSES biases efficient: the images of PWR SST – CMC are noticeably more uniform than the images of BSST – CMC. Note that comparison with CMC L4 in Fig.1 independently verifies the LUT derived from *in situ* data shown in Table 1 (from 15 May 2013 – 8 August 2014), in a global domain, and for the data outside the training time interval.

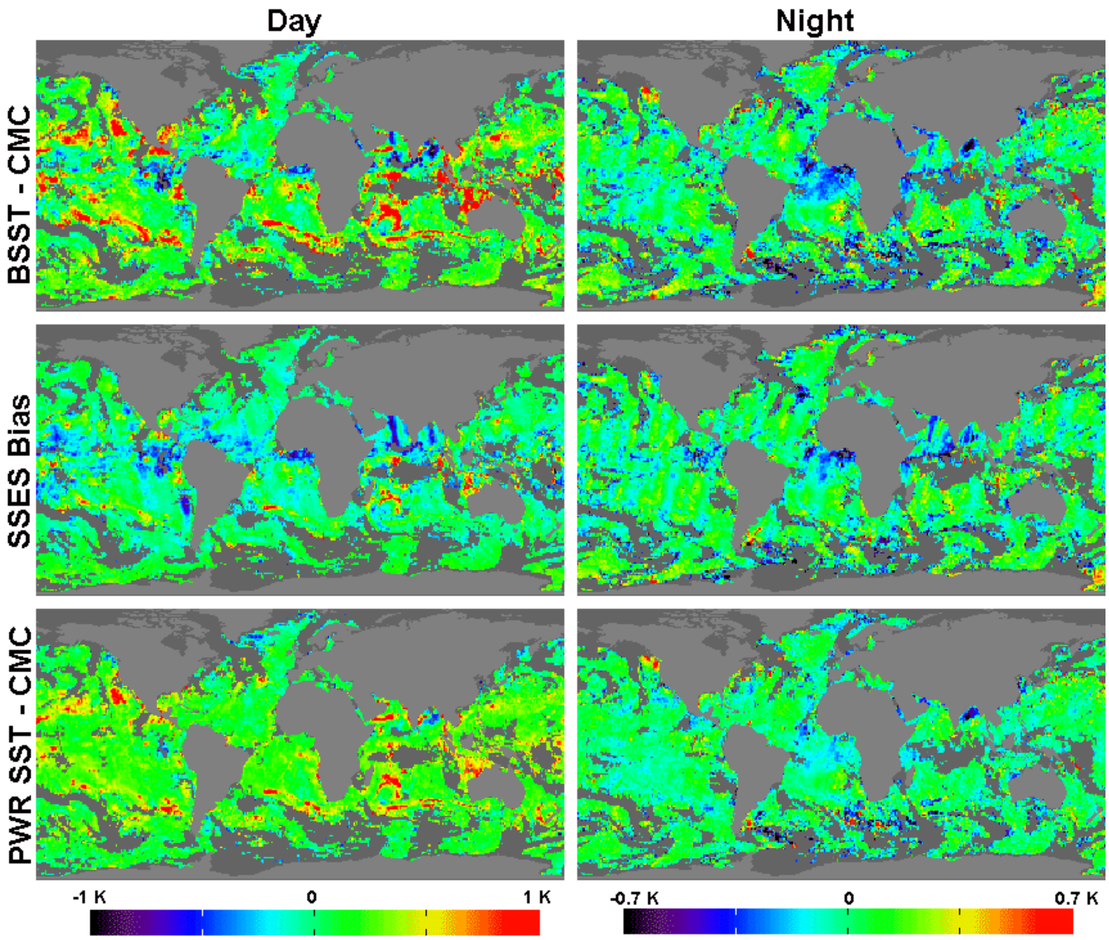

Fig.1. (Left panels) daytime and (right panels) geographical distributions of (top) BSST – CMC SST, (middle) SSES bias, (bottom) PWR SST - CMC SST from S-NPP VIIRS observations on 16 February 2015.

Fig.2 shows time series of daytime biases and SDs of BSST, PWR SST and CMC with respect to *in situ* SST, for six satellite sensors from 24 November 2014 to 10 March 2015. (Note that this is an independent verification of the LUT derived from the 15 May 2013 – 8 August 2014 data set and used for training of the PWR SST coefficients.) The statistics for all three SSTs were estimated from daily matchups and smoothed with a 7-day time window. Comparison of the BSST and PWR SST shows that the SSES bias correction makes the statistics more stable and consistent between the sensors. It also reduces the peak-to-peak range of variations in the global SDs from ~0.35-0.52 K for BSST to ~0.27-0.38 K for PWR SST. Fig. 2 also shows the difference in daytime CMC biases for different sensors caused by the diurnal surface warming. The CMC biases are close to zero for the MetOp-A and -B whose equator crossing time (ECT) is 9:30 am, several hundredths of K colder for Terra, whose ECT is 10:30am, and close to - 0.2 K for the S-NPP, Aqua and NOAA-19, which cross the equator around 1:30 pm. The PWR SST brings global daytime SDs closer to the level typical for CMC but produces much more consistent biases, for all platforms. This may suggest the benefit of assimilating the daytime PWR SST into L4 analyses (recall that daytime SSTs, especially with low winds, are often excluded from L4 analyses), or even creating a “daytime” L4 SST product (whose performance based on our analyses is expected to be comparable with the L4 SSTs produced from nighttime SST retrievals).

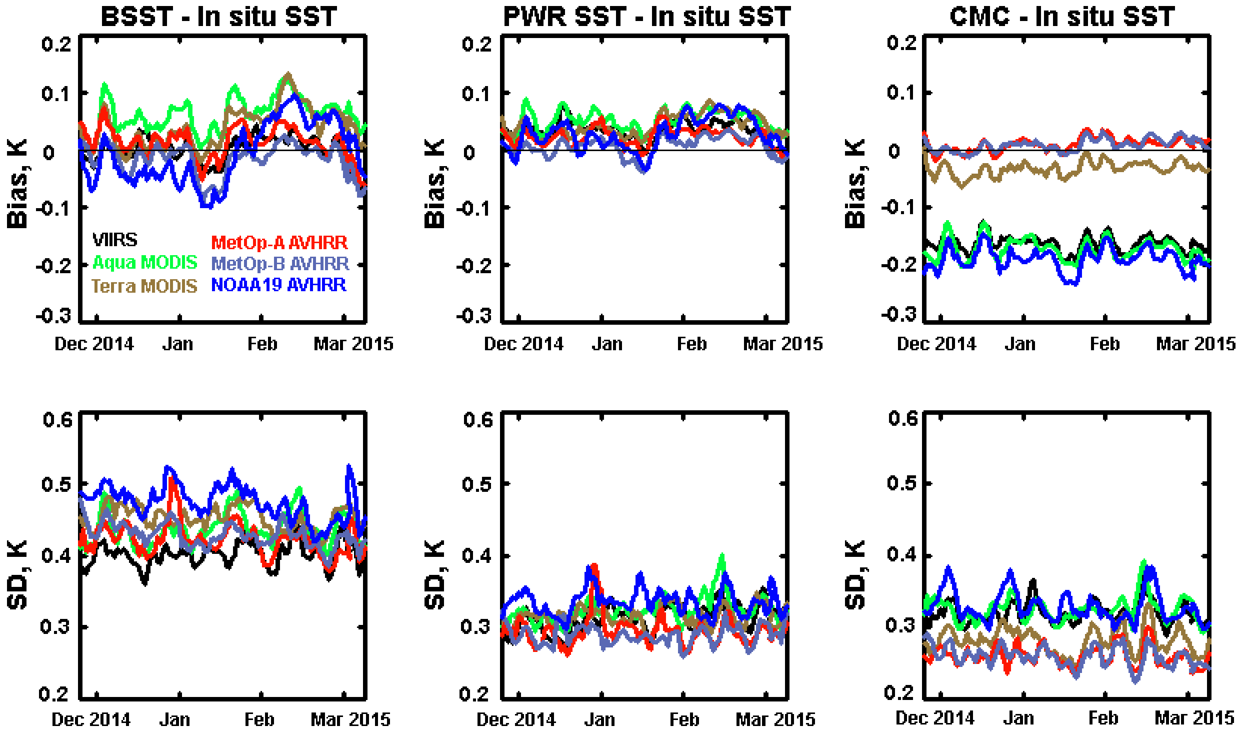

Fig. 2. Daytime time series of daily global biases and SDs of fitting in situ SST with BSST, PWR SST and CMC, for six satellite sensors, from 24 November 2014 to 10 March 2015.

4. Summary and conclusions

The redesigned ACSPO SSES algorithm performs segmentation of the SST retrieval domain in the space of regressors deriving the segmentation parameters from the statistical structure of regressors within the training MDS. SSES biases are calculated as differences between the BSST and the PWR SST estimated with coefficients specific to each segment. Applying SSES biases defined this way results in significant reduction in the global SDs of fitting the *in situ* SST with PWR SST, compared to the BSST.

Thus, ACSPO v2.40 provides the PWR SST, in addition to the BSST. The PWR SST is not represented in the output ACSPO files as a separate layer but can be obtained by subtracting the SSES bias from the BSST. The two products have different features. The BSST provides a reasonable combination of precision with respect to *in situ* SST and sensitivity to “skin” SST (Petrenko et al., 2014b). As such, it is considered the “skin” SST product (although trained against *in situ* SST). The PWR SST, on the other hand, fits *in situ* SST much more precisely than the BSST. Therefore, it may be considered an estimate of the “depth” SST. Currently the PWR SST undergoes a comprehensive testing and, depending on results and users’ feedback, it may be designated as a standalone "depth" product in the subsequent versions of ACSPO.

A full range of potential applications of PWR SST is yet to be determined. In particular, it is expected to benefit producers of the “foundation” L4 SST, by reducing (or even eliminating) the need in the L4-specific “bias correction”. The fact that the daytime PWR SST has global precision comparable with that of L4 SST, but is not biased cold with respect to *in situ* SST, may suggest the possibility of assimilating daytime ACSPO SSTs into the current L4 analyses, or even creating a new “daytime” L4 SST.

The SSES SDs in ACSPO v.2.40 are calculated for each segment as SDs of BSST minus *in situ* SST. The performance of the new SSES SD has not been evaluated yet. This could be done by using the SSES SDs for weighting BSST differently than the *in situ* SST, during their assimilation into the L4 analyses. Note that the SDs for the PWR SST are not currently reported because the GDS 2.0 format does not allow for two SSES statistics. However, it may be easily added to the ACSPO output per users’ request.

Note that no special effort was made in ACSPO 2.40 to provide a seamless connection between the values of PWR SST at the boundaries of different segments. As a result, the PWR SST images may include some discontinuities. Our analyses show, however, that such artifacts are typically small enough, rarely reaching several tenths of a degree Kelvin, and should not affect the L4 analyses which assimilate the L2/L3 data and perform additional smoothing in space and/or time. This problem will be addressed in the future versions of ACSPO. In the meantime, caution is advised in analyzing the SSES corrected SST imagery using data of ACSPO 2.40.

5. Acknowledgments

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