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14. ABSTRACT

Worked on estimation of sea surface temperature (SST) from satellite infrared imagery and its applications to numerical weather forecasting and as means to reduce noise in satellite data retrievals influenced by skin SST diurnal effects). Flatau observed significant contributions to the local standard deviations of SST which are due to total precipitable water (PW) bias particularly for large PW contents of the order of 4-7 cm in tropics.

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N00173-09-1-G905 - Sea Surface Analysis in Support of the NRL NWP Modeling

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Summary

We report on our work on estimation of sea surface temperature (SST) from satellite infrared imagery and its applications to numerical weather forecasting and as means to reduce noise in satellite data retrievals influenced by skin SST diurnal effects). Current approach is based on the Advanced Very High Resolution Radiometer (AVHRR) on the first Meteorological Operational satellite (Metop-A) and NOAA19 as well as NOAA18 matched in time and space to the fixed and drifting buoy surface SST. The basic state fields are based on analyzed atmospheric fields from the NRL Monterey NOGAPS global numerical weather prediction system, the forward and inverse model interface to both CRTM and RTTOV were developed. A reduced state vector comprises of skin SST, total column water vapor as well as atmospheric temperature and ozone. Operational SST retrievals from NAVOCEANO are used and the relevant dataset is described. The SST data stream contains BT temperatures in Channels 3-5, satellite geometry, fixed and drifting buoy matchups. We observe significant contributions to the local standard deviations of SST which are due to total precipitable water (PW) bias particularly for large PW contents of the order of 4-7 cm in tropics. Using linear empirical bias corrections provides method to reduce retrieved top of the atmosphere brightness temperature minus AVHRR observed BT.

1. NAVOCEANO SST data files

1.1. Global data

The Naval Oceanographic Office national SST product (May, Parmeter, Olszewski, & McKenzie, 1998) consists currently of about 500,000 global retrievals per day for one satellite. A complete overview of the national Shared Processing Program (SPP) satellite sea surface temperature (SST) retrieval product is beyond the scope of this document. However, same relevant aspects of the operational processing of digital Advanced Very High Resolution Radiometer (AVHRR) satellite data into a global SST retrieval product at the Naval Oceanographic Office (NAVOCEANO) is described here. The data set exist for NOAA-18 and METOP-A AVHRR GAC. The files are in a protected area on the GODAE server. For this report several date time group files (DTG) were examined. The standard data type codes for SST are 151, 152, 159 which stand for day, night, and relaxed conditions. The aerosol flagged type codes are 161 and 162. The data includes buoy match-up files with the same information but collocated in space and time with the drifting buoys. These files will provide us some ground truth information along with the orbital swath satellite data. Either file can be read in FORTRAN as blank delimited, list input. At NAVOCEANO a script is run once a day and delivers the previous day's SST retrievals (global files) and the SMDB (SST Matchup Database files) matchups from current day minus two. The SMDB files contains one day of data. The GLOBAL dataset may contain about 500,000 observations a day and matched SMDB data contains about 5000 data points.

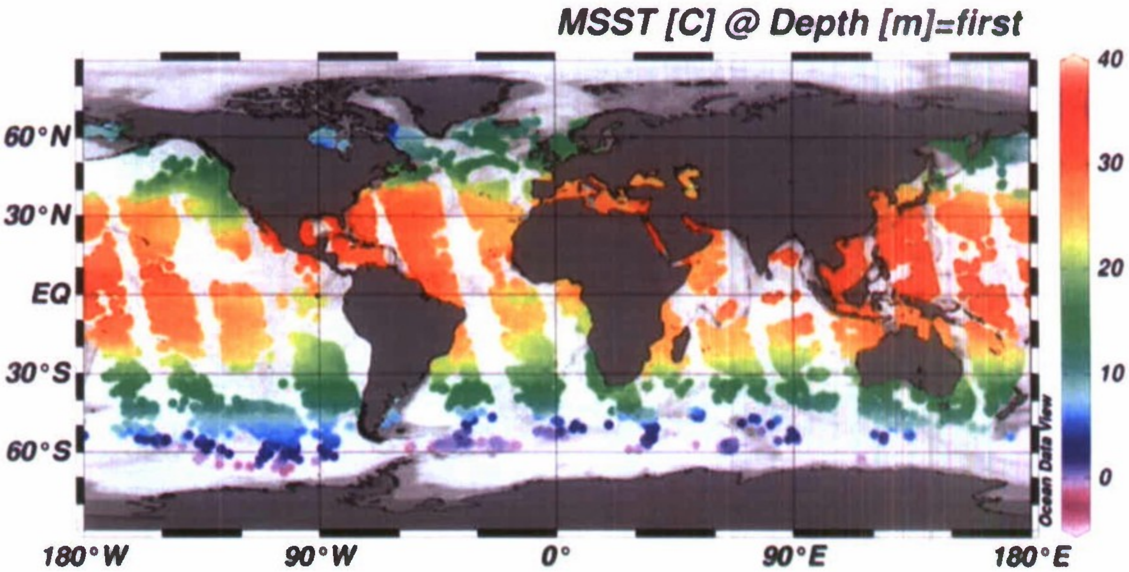

Figure: Metop-A SST retrievals using NLSST algorithm from the Naval Oceanographic Office on August 15, 2009. Only type=152 (night) SSTs are presented. Every 10^{th} point is plotted.

SST files are described in Table.

Variable	Explanation
Type	151, 152, 159 = SST day, night, relaxed day
Type	161, 162 = SST possible aerosol contamination day and night
yr4d	Year
Mnth	Month

Daym	Day
Hour	Hour
Minh	Minute
Secm	Second
Lati	Latitude
Loni	Longitude
Msst	retrieved SST
Reli	RMS values from our matchups
Soza	solar zenith angle
Saza	satellite zenith angle
Fsst	100km field SST
Bias	bias values from our matchups
Soaa	solar azimuth angle
Csst	climatological SST
Clas	category (1 = clear, 2 = probably clear, 3 = possibly cloudy)
ac1a ac2a	channels 1 and 2 reflectance values
ac3a	channel 3a reflectance or channel 3b brightness temps (looks like 3a/3b switch is occurring in MetOp, but not in N-18 which is just 3b)
ac4a ac5a	channel 4 and 5 brightness temperatures

1.2. SST Matchup Data Base and QC

SMDB (SST Matchup Data Base) files include the SST variables above plus several variables describe in Table. In the original data stream all matchups available in each SMDB are included which means that there can be multiple buoy matchups for an individual satellite SST.

The SST matchup database contains drifting and moored buoy SSTs and satellite SSTs that are matched within time and distance constraints of 4hr and 25km. Global drifting buoy, Tropical Ocean and Global Atmosphere program Tropical Atmosphere Ocean array moored buoy, and Pilot Research moored array in the Tropical Atlantic SST measurements received through Global

Telecommunication System and DOD communication lines are used in the match process. The buoy quality control measures have not been performed on the data that we are receiving at present and there is no filtering of the matchup data. In NAVOCEANO additional QC of matchup data is performed during regression step (Douglas May, personal communication, file "navoceano buoy matchup statististicsv2.doc"). We are also screening ship/buoy dataset for deviations from a climatology (on the basis of tests with climatological and 100km SST) and remove duplicate matchup. The following if/then statement is used to screen out buoys that are reporting inaccurate temperatures or are located in frontal regions: if (abs(buoy-climo) .le. 1) or (abs(buoy*2-climo-fld) .le. 3) then if (abs(sst-buoy) .lt. 4) proceed. The field values (fsst) are obtained from a 100km analyzed temperature field generated daily by objectively analyzing all satellite SST retrievals collected during the past 36hr using a 1 degree latitude-longitude grid. The climatology values are obtained from a 1 degree resolution (lat/long grid) hybrid climatology file that is updated daily. The file contains NMC (National Meteorological Center) Adjusted OI climatology from 70S to 70N and NCAR (National Center for Atmospheric Research) 20-year climatology from 70N to 80N.

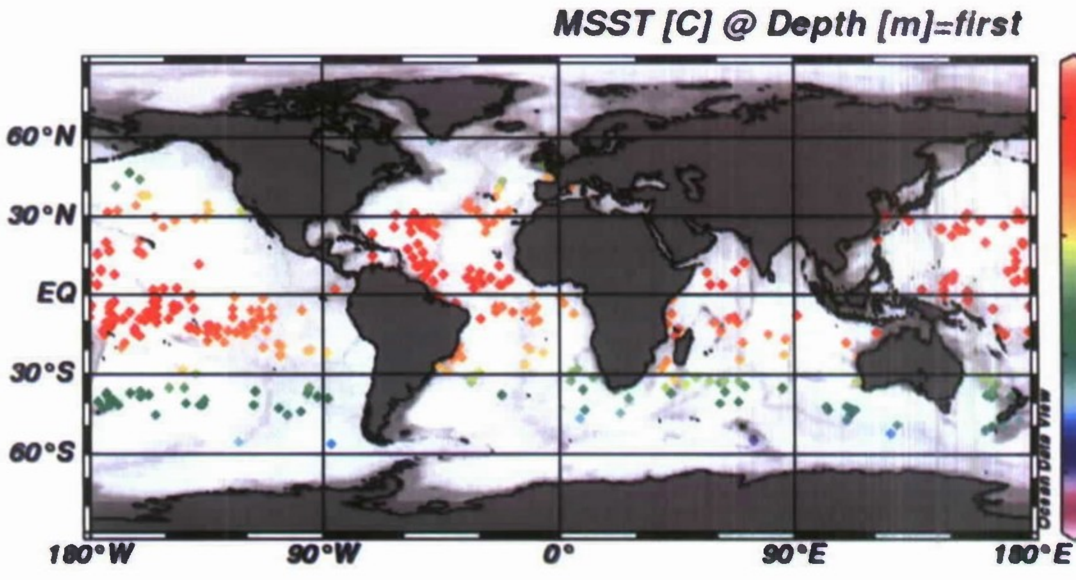

Figure: Quality controlled matchup cases for Metop-A SST retrievals using NLSST algorithm from the Naval Oceanographic Office on August 5, 2009. Day and night are both incuded.

Variable	Explanation
Srce	105 = fixed buoy 106 = drifting buoy
Year Mnth Daym Hour Minh	matchup time
Lati	Latitude
Loni	Longitude
Ssst	buoy SST
Ship	buoy ID
Mind	distance in km of buoy sst and satellite SST match
Hrmt	difference in hours of the matchup

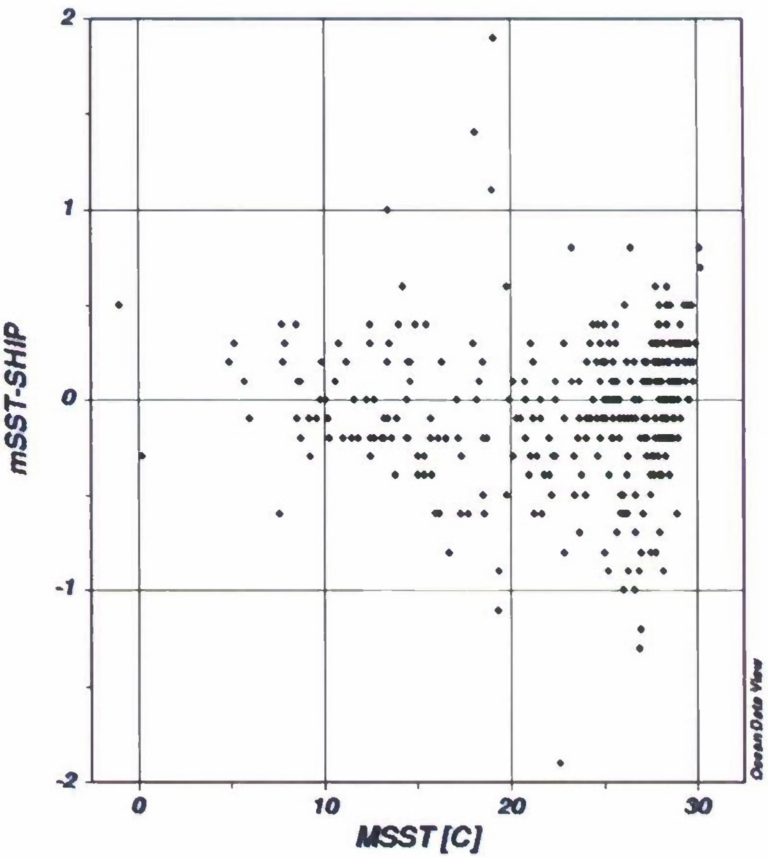

Figure: Metop-A SST retrievals using NLSST algorithm subtracted from buoy matchup (mSST-SHIP) as a function of mSS for August 5, 2009. Day and night cases are presented after quality control criteria (for example, comparison with climatology and SST gradient) described in the text were applied as well as cloudy points were removed.

1.3. Daytime SST Processing and Algorithm

To provide basic understanding of the SST algorithm we provide abridged daytime SST processing algorithm on the basis of the NAVOCEANO unpublished technical note (Douglas May, NAVOCEANO, personal communication, file seatemp processing 01dec05.doc) . Much of details are removed. However, assumption important for physical retrievals such as satellite and solar zenith angle flags, cloud clearing flags, as well as land-sea mask are discussed in some detail as they are of importance for the physical retrievals as well.

Step	Description
Daytime/Nighttime Test	Daytime data is determined by checking that Solar Zenith angle (solz) ≤ 75 degrees.
Satellite Zenith Angle Test.	Check of satellite zenith (satz) angle is performed. Only satz ≤ 53 degrees are accepted.
Gross Cloud Test.	
Land/Sea Test.	The land mask contains a distance from land value for each 1km grid cell. SST retrievals are made within 4km of land at nadir (satellite geopositioning is no better than plus or minus one pixel). This value is automatically adjusted according to satellite zenith angle to account for spatial resolution changes along scan. The processing distance from land changes

	according to the following formula: distance = 4km / cos(satzen)**2.
Channel 4 Gross Cloud Test.	Check that (270K ≤ C4 ≤ 310K).
Channel 5 Gross Cloud Test.	Check that (268K ≤ C5 ≤ 310K).
Visible Cloud Threshold Test.	
Channel 2 Uniformity Test.	
Channel 4 Uniformity Test,	
Channel 5 Uniformity Test.	
Reflected Ratio Test.	
SST Intercomparison Test.	Check that ABS(NLSST – MCSST) ≤ 1.5 using 2x2 pixel average values.
Unreasonable SST Test.	Check that (-2 ≤ NLSST ≤ 35), using 2x2 pixel average values.
Climatology Test.	Check that (ABS (NLSST-CLIM) ≤ 10) using 2x2 average values. CLIM is the closest global climatology field value to the retrieval lat/lon. If CLIM is invalid (some coastal locations) then use MCSST as CLIM

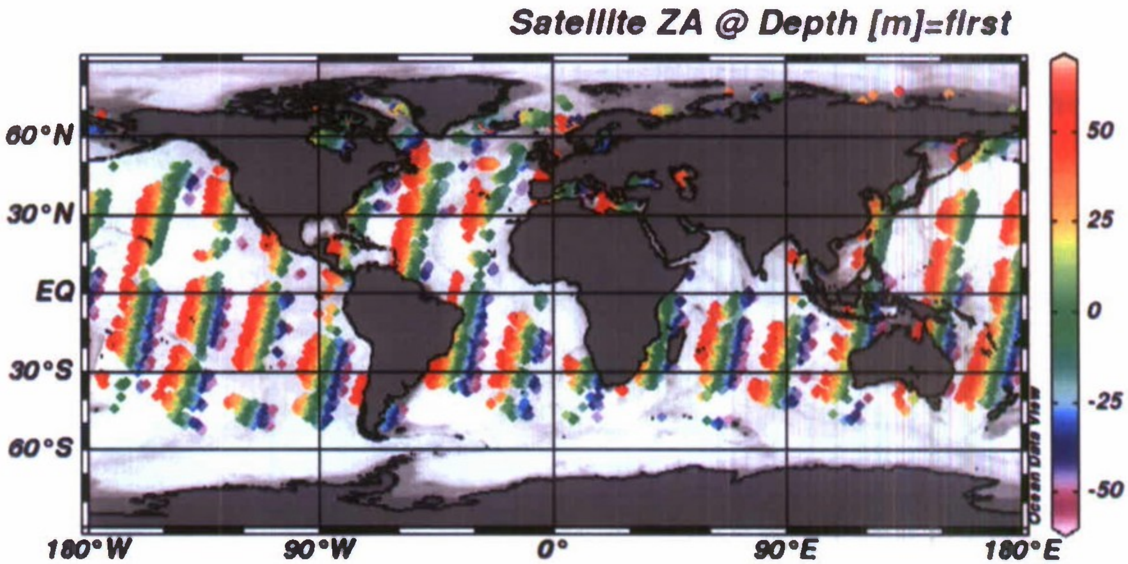

Figure: Metop-A satellite zenith angle is limited to -53, 53 degrees. Here, only day overpasses are presented.

1.4. The NAVOCEANO SST algorithm

The NAVOCEANO SST algorithms are based on the following expressions

NLSST = a1*C4 + a2*FLD*(C4-C5) + a3*(C4-C5)*(sec (0)-1) – a4

Where FLD is the closest 100km analyzed SST field value to the retrieval lat/lon, C4 and C5 are 2x2 average values. Sec (0) is secant of the satellite zenith angle (satz).

MCSST= a1*C4 + a2*(C4-C5) + a3*(C4-C5)*(sec (0)-1) – a4. If FLD is invalid (some coastal locations) then use MCSST as FLD, where a1, a2, a3 and a4 are empirical constants.

In operational mode the non-linear NLSST algorithm is used and it is based on channel 4, 5 during the daytime and channels 3, 4, 5 during the nighttime.

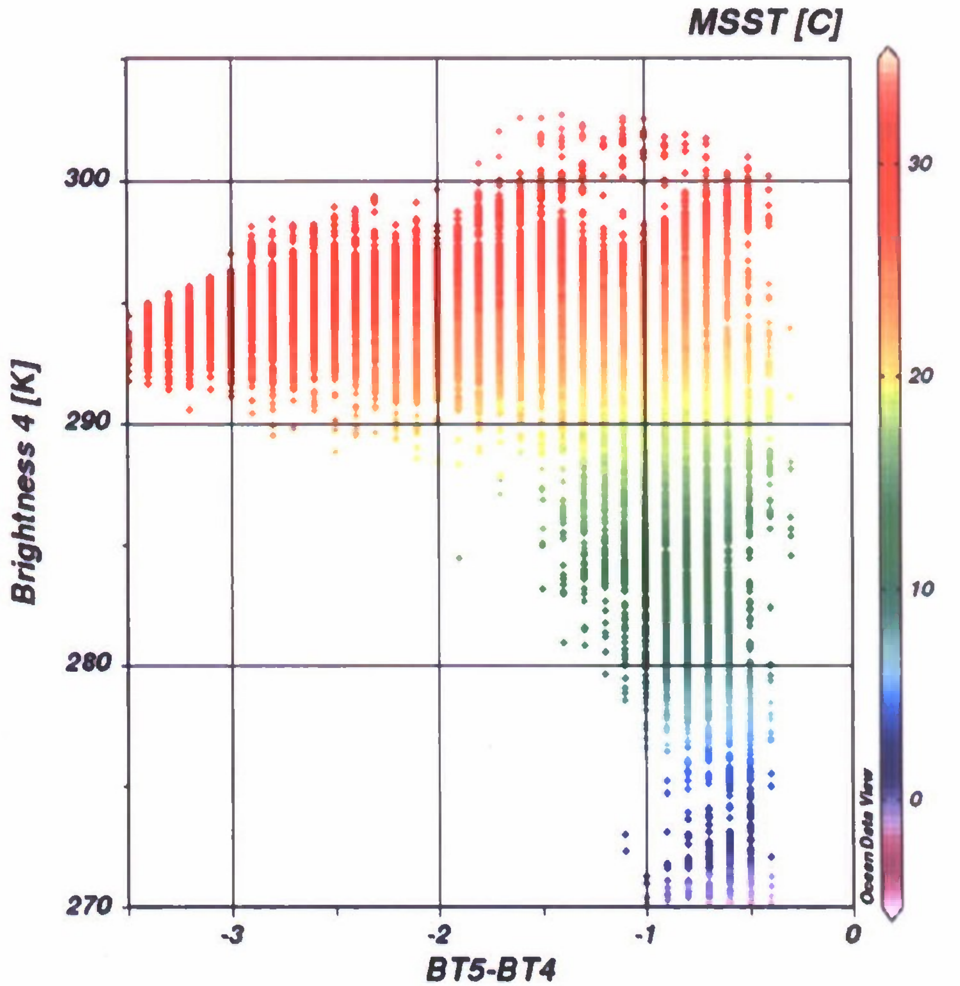

Figure: Brightness temperature difference (split window) in Channel 5 and 4 as a function of brightness temperature in channel 4. Non-linear SST retrievals are presented on this figure. Metop-A satellite night data are selected for August 15, 2009.

2. NRL models - radiative transfer codes interface.

Current interface between radiative transfer models and Naval Research Laboratory atmospheric global model is through dataset employed every 6 hours by the Navy Aerosol Analysis and Prediction System (http://www.nrlmry.navy.mil/aerosol) model. This model is driven by meteorological fields obtained from the Navy Operational Global Atmospheric Prediction System (Hogan & Rosmond, 1991). NOGAPS uses a hybrid sigma-pressure coordinate system with terrain-following sigma surfaces near the ground transitioning to constant pressure surfaces near the top of the domain to1 hPa. Current operational NOGAPS resolution is T239 (~0.5 degree on the Gaussian grid). The NOGAPS latitude-longitude data is on regular 720x360 grid. We use 30 vertical layers (with pressure pcenter)and 31 vertical levels (on pressure p). The NOGAPS data is decompressed and matched with satellite observations over the ocean to form an initial state vector which contains information about the atmospheric and surface state as well as top of the atmosphere radiances. The Table describes list of variables which are used to form profiles. Ozone profile climatology is not forecasted in NOGAPS and is taken from climatology.

Variable	Description
lon	Longitude
lat	Latitude
terrain	Terrain height [meters]
oceann	Ocean fraction [0..1]
xland	Land fraction [0..1]
seaicen	Sea ice fraction [0..1]
glacier	Glacier fraction [0..1]
dragst	Surface stress [kg/m/s]
lheast	Laten heat flux [W/m^2]
sheast	Sensible heat flux [W/m^2]
stst	Surface temperature in [K]
swst	Surface wetness fraction [0..1]]
snowst	Snow temperature [K]
cprec	Cumulus precipitation [mm]
sprec	Stable precipitation [mm]
pclclo	LCL [mb]
cumtopo	Cumulus top [mb]
cufraco	Cumulus fraction
spst	Surface pressure [mb]
u, v	Surface horizontal velocity [m/s]
RH(maxk)	Relative humidity at layer pressure RH=100. sh/qsat [0..100]
Sh(maxk)	Specific humidity at layer pressure

T(maxk)	Air temperature at layer pressure [K]
P(maxk+1)	Pressure at levels converted from sigma coordinates (p=asig+bsig*spst)
Pcenter(maxk)	Pressure at midpoint between two layers (pcenter= ½ ((asig+ asig+) + (bsig + bsig+) spst)
wvpath	Water wapor path = (1./cos(saza) integral (q dp) /g, where q is specific gumidity

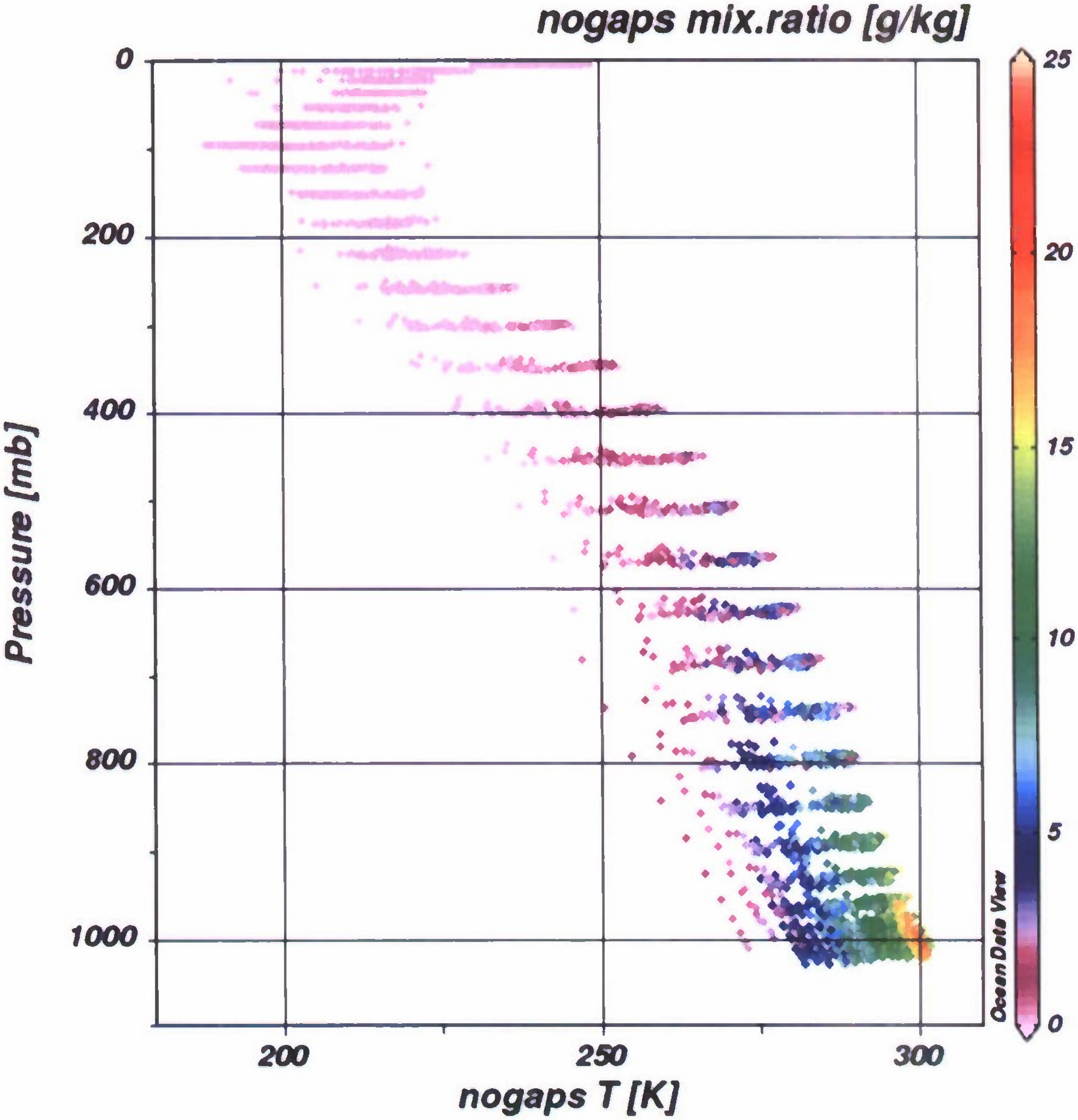

Figure. NOGAPS vertical temperature distribution as a function of pressure and water vapor mixing ratio [g/kg] only for soundings matching the buoy data at night on August 5, 2009. Water vapor content and its vertical distribution are variables which controls brightness temperature in the AVHRR IR window.

3. Forward model brightness temperature estimates

3.1. Introduction

We use 2 radiative transfer codes to simulate radiances at the top of the atmosphere: (a) community radiative transfer model (CRTM) developed in support of Joint Center for Satellite Data Assimilation (JCSDA) and the RTTOV model developed under cooperation between EUMETSAT, the Met Office, UK, and by other partners. These codes have similar functionality in our applications. However, the calling sequence and tests performed on model input are somewhat different in both cases. Also, the codes have been largely developed independently. This makes it valuable to employ on occasion both models for validation as well as more practical task of removal of state vectors beyond training set of the RT models.

3.2. Community radiative transfer model (CRTM)

Community radiative transfer model (CRTM) was used to simulate radiance at the top of atmospheres for NOAA-18, NOAA-19, and Metop-A satellites. This model (Liang, Ignatov, & Kihai, 2009) was developed by efforts of the Joint Center for Satellite Data Assimilation (JCSDA). The CRTM source code and coefficients, and example programs, were obtained via the ftp site ftp://ftp.emc.ncep.noaa.gov/jcsda/CRTM/ and documented in NOAA Technical Report NESDIS 122, JCSDA Community Radiative Transfer Model (CRTM) - Version 1, Yong Han, Paul van Delst, Quanhua Liu, Fuzhong Weng, Banghua Yan, Russ Treadon and John Derber, 2006, Washington DC, 2005. The CRTM libraries were build on linux using gfortran compiler. Forward calculations of the top-of-atmosphere (TOA) radiances and brightness temperatures for an input atmospheric profile were calculated for the AVHRR sensor on Metop-A for channels 3,4,5 (CH3 BT, CH4 BT, CH5 BT). Atmospheric structure was assigned by defining level pressure and layer pressure obtained from NOGAPS. Two atmospheric absorbers were specified – water vapor and ozone mixing ratio. Clouds and aerosols were not defined. Above pressure of 1 mb soundings were extended using the US Standard Atmosphere climatology. Ozone mixing ratio, was also set to climatology and kept the same for all times and all locations. Surface type was defined as sea water and surface temperature set to the NAVOCEANO mSST. Satellite geometry was defined by sensor zenith angle and scan angle and were both set to be the same and that given by satellite zenith angle. Atmospheric profile was defined on the basis of satellite position and no account for the slant path was considered. One profile and one sensor were calculated for each call to the CRTM.

3.3. Radiative Transfer for (A)TOVS (RTTOV)

The RTTOV model (Saunders, Matricardi, & Brunel, 1999) was developed under cooperation between EUMETSAT and the Met Office, UK, by other partners. We used RTTOV9.1 version of the model. The model allows for rapid simulations of radiances of satellite infrared scanning radiometers given an atmospheric profile of temperature, variable gas concentrations, cloud and surface properties. The only mandatory variable gas for RTTOV9.1 is water vapor but we also define ozone profile based on climatology. RTTOV9.1 can accept input profiles on any set of pressure levels. Temperature, water vapor mixing ratio, and pressure are defined at 2m based on NOGAPS atmospheric data. Horizontal velocity at 2m is set to zero. Skin SST is defined as mSST. Satellite zenith angle, satellite azimuth angle is set to 0, solar zenith and azimuth angles are set according to NAVOCEANO data stream. No clouds or aerosol effects are taken to account. Pressure is defined for atmospheric layers (center of pressure levels).

3.4. CRTM vs. RTTOV intercomparison

Figure below presents channel 5 brightness temperature differences between the CRTM and RTTOV models as a function of satellite zenith angle. The total water vapor in atmospheric slant path in [g/kg] is used to label the data. State vector is based on the NOGAPS prediction for the night of on August 5, 2009. The differences between the models are overall fairly small in the (0.2K). However, there is clear dependence on satellite zenith angle. Some of the differences are reaching 0.4-0.8K for large satellite zenith angles and small water vapor. It is not clear what the reasons for these deviations are. However, it indicates that the satellite zenith angles need to be constrained in SST retrievals to about 40 degrees to reduce RT model biases to approximately 0.2K. In addition the CRTM code does not provide, at present, an easy way to flag state vectors beyond its molecular properties database training set. The RTTOV code offers such option. Therefore, we remove all cases of atmospheric soundings flagged as erroneous by the RTTOV.

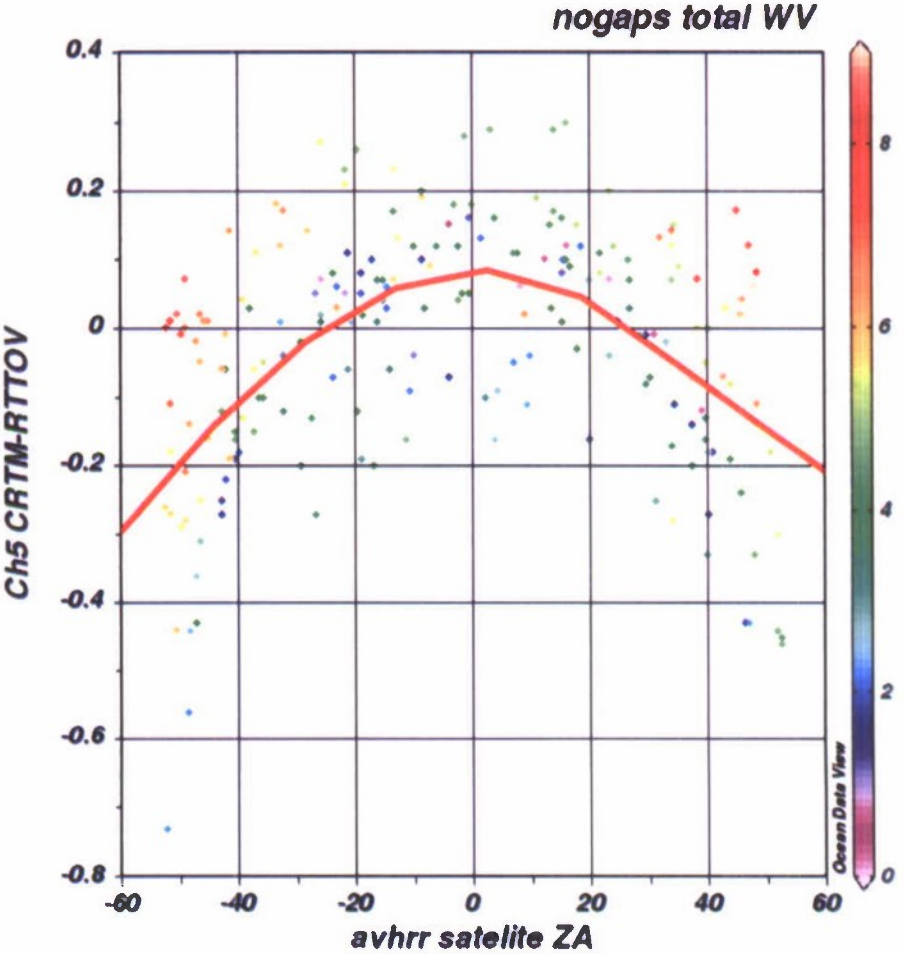

Figure. Channel 5 brightness temperature differences between the CRTM and RTTOV models as a function of satellite zenith angle. Total water vapor in atmospheric slant path in [g/kg] is used to label the data. State vector is based on the NOGAPS prediction for the night of on August 5, 2009.

3.5. SST physical retrieval algorithm

There are several codes which are used to convert data stream and calculate radiances. These codes are written in Fortran95 and are briefly described below.

Code	Description
convert	NOGAPS/NAAPS converter form custom NAAPS packed binary to IEEE binary. Additionally, pressure at layers center "pcenter" and RH are calculated. Model data is converted from the hybrid sigma layers. Input: NOGAPS compressed, Output: NOGAPS IEEE binary
smdb	Reads in NAVOCEANO data (-2 days) and performs quality control of ship data

	including tests of temperature frontal zone and deviations from a climatology. Multiple matches for the same station are removed. Only cloud free cases are retained. Additional flags include limits of DTG group and sun zenith angle. gfortran smdb2.f90 –o smdb2 ./smdb2 smdbMTArelax_05AUG09.txt all 0 24 90 Output: smdb.txt
merge	Merges NOGAPS data and satellite data to form a profile. gfortran merge.f90 -o merge ./merge 20090825005x5.bin smdb.txt Output: profile.txt
rtc	Invokes radiative transfer calculations (CRTM/RTTOV) to calculate TOA brightness temperature on the basis of "a profile" (state vector). Makefile links with crtm and rttov libraries ./crtm Input: profile.txt, Output: odv.txt

3.6. Results

Recently several attempts were reported in the literature of optimal estimation (OE) of sea surface temperature estimated from satellite infrared imagery in the "split-window", in comparison to SST retrieved using the usual multi-channel (MCSST) or non-linear (NLSST) estimators. In one case (Merchant, Le Borgne, Marsouin, & Roquet, 2008) the prior state vector for the OE was based on forecast atmospheric fields from the Météo-France global numerical weather prediction system (ARPEGE) and the forward model radiative transfer model was RTTOV8.7. They used a reduced state vector comprising of SST and total column water vapor. Significant contributions to the global standard deviation arisen from regional systematic biases of several tenths of kelvin in the non-linear SST regression (NLSST) algorithm. Simple empirical bias corrections to improve the OE by changing total water vapor content were investigated. Similar approach was undertaken (Tomazic & Kuzmic, 2009) using the European Centre for Medium-Range Weather Forecast (ECMWF) ERA-40 reanalysis dataset. This dataset provided the temperature and humidity profiles and surface data, while the RTTOV 8.7 radiative transfer model was used to calculate the top-of-atmosphere brightness temperatures for the advanced very high-resolution radiometer (AVHRR) channels. Ten ERA-40 grid points over the Adriatic Sea were used in the analysis. It was shown that SST retrievals are improved when considering regional atmospheric state vector. Similar effort is also reported by NOAA (Liang, et al., 2009) who use fast Community Radiative Transfer Model in Advanced Clear-Sky Processor for Oceans (ACSPO). CRTM is used in conjunction with the National Centers for Environmental Prediction Global Forecast System atmospheric profiles and Reynolds weekly version 2 sea surface temperatures to simulate clear-sky brightness temperatures.

Our approach uses NOGAPS state vectors, RTTOV and CRTM radiative transfer models, NAVOCEANO matched NOAA18, NOAA19, and Metop-A dataset. As an example we present channel 5 brightness temperature differences between the CRTM model and AVHRR observations on METOP-A as a function of slant path water vapor are presented on Figure below. State vector is based on the NOGAPS forecast for the night of August 5, 2009. Red line is a least square fit. Two cases are presented (a) uncorrected NOGAPS total water vapor path, (b) retrievals based on linearly corrected total water vapor. This correction amounts to over prediction of columnar water vapor amount by about 25% at 7g/kg columnar water vapor and 0% at 3g/kg. The correction was applied uniformly throughout the atmospheric column.

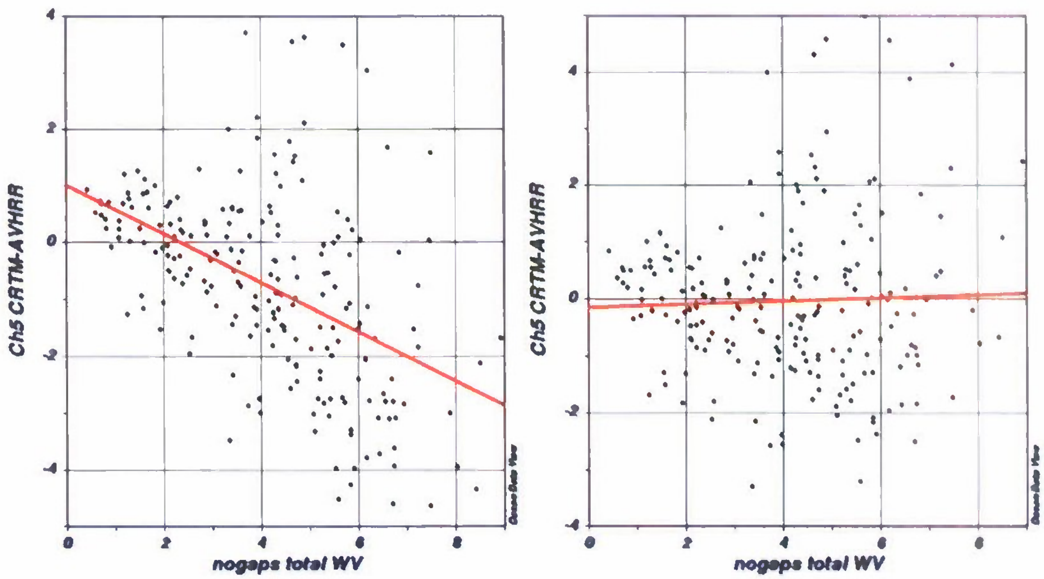

Figure. Channel 5 brightness temperature differences between the CRTM model and AVHRR observations on METOP-A as a function of slant path water vapor. State vector is based on the NOGAPS prediction for the night of August 5, 2009. Red line is a least square fit. (a) uncorrected NOGAPS total water vapor path, (b) retrievals based on linearly corrected total *water vapor. This correction amount to over prediction of columnar water vapor amount by about 25% at 7g/kg columnar water vapor and 0% at 3g/kg.*

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