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Compilation of a High Resolution Sea Surface Temperature Dataset from Satellite Measurements for the Gulf of Mexico

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1. INTRODUCTION

The purpose of this task is to develop a high-resolution sea surface temperature (SST) dataset to be employed in meteorological modeling using the Penn State University (PSU)/National Center for Atmospheric Research (NCAR) Fifth Generation Mesoscale Modeling System (MM5) [Grell et al., 1996]. The meteorological fields from MM5 will be used as part of a standard dataset to drive the CALPUFF dispersion modeling system [Scire et al., 2000a, b] in offshore and coastal applications in the Gulf of Mexico area. We present here a brief background on the need to have a high-resolution sea surface temperature data in meteorological modeling. In the following sections, we also discuss the approach taken in arriving at a daily SST dataset from high-resolution satellite measurements.

Modeling the air quality impacts from sources offshore or in coastal areas is often influenced by mesoscale circulations such as the land/sea breeze. In addition, dispersion properties of the atmosphere offshore are typically quite different than those over land, making knowledge of the marine boundary layer structure critical for dispersion modeling for these sources. Coastal sites often experience a land/sea breeze circulation that exhibits a diurnal pattern with weak offshore winds at night and strong onshore winds during the day. This is in association with the diurnal heating and cooling of the landmass adjacent to the coastal water body.

Sea breezes are a mesoscale phenomena occurring on spatial scales between 1 and 200 kilometers (km). Owing to these spatial scales, coarse-scale numerical weather prediction models may not properly characterize detailed sea breeze circulations. Mesoscale meteorological modeling using models such as MM5 is often needed to accurately simulate these effects. More modeling work is needed to fully understand the meteorology of complex coastal environments [Cai et al., 2000; Rogers, 1995].

One key input to meteorological models simulating sea breeze circulations is the SST. Sea breeze strength and penetration depends on the difference between the air density over land and that in the marine layer. The properties of the marine layer strongly depend on the temperature at the surface of the underlying ocean. Hence, the larger the difference between the land temperature and the neighboring SST, the stronger will be the tendency for a sea breeze. As indicated previously, the sea breeze flows are of an order of a few kilometers to a few hundred kilometers. This requires that the spatial resolution of the available SST data be between these scales in order to accurately model the sea breeze effects.

SST data is currently available on a variety of spatial and temporal scales. Details about the source and scales of the SST data are presented in Table 1.

The purpose of this task is to compile a SST data on a resolution of ~36 km and ~4 km (at the equator) employing the Moderate Resolution Imaging Spectroradiometer (MODIS) measurements.

2. DATA COMPILATION

2.1 MM5 Modeling

Under separate contract to the Minerals Management Service (MMS), Sonoma Technology, Inc. (STI) and PSU will run the MM5 meteorological model at 36km/12km/4km nested grid meshes for the period October 1, 2000 to September 30, 2001. This provides the standard three-dimensional meteorological dataset for use in dispersion modeling with CALPUFF. The SST data that will be used to force the lower-boundary in MM5 is being prepared by Earth Tech. under a contract with the MMS. As a reference, we have included the STI/PSU modeling domain for MM5. This is presented in Figure 1.

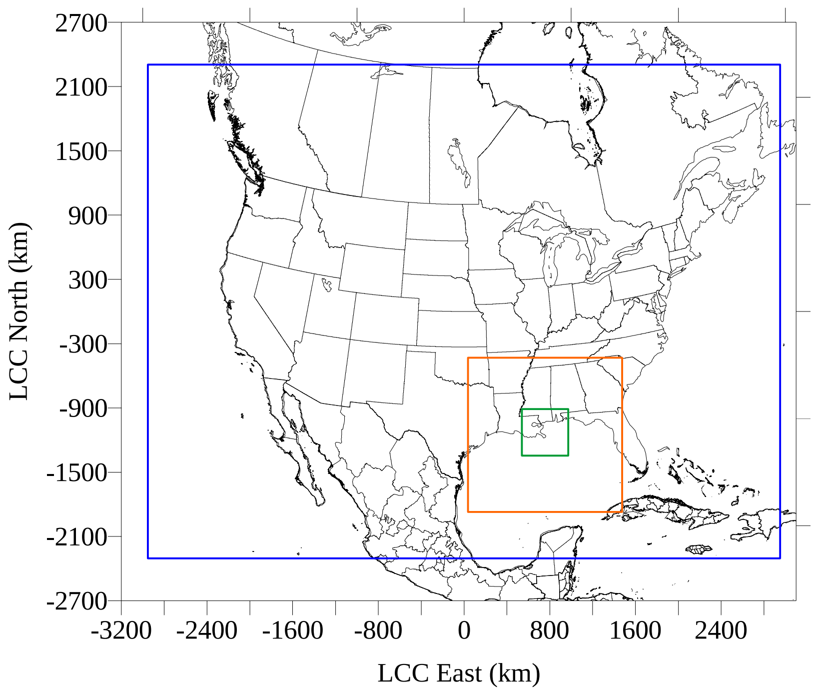


Figure 1. MM5 modeling domains to be used in providing the standard meteorological data for use with the CALPUFF model. The blue, orange, and green boxes represent the three domains that will be used by STI/PSU.

Briefly, there will be three domains employed in the MM5 modeling. The outer domain covering the whole United States will be at a 36 km grid spacing, while the inner two over the Gulf of Mexico and New Orleans would be at 12 and 4 km grid spacings, respectively. Further details about the model parameters and physics options can be obtained from the report from STI.

We prepared SST data over the United States at two resolutions. One at ~36 km grid spacing for the whole United States (for Domain 1) and the other at ~4 km grid spacing over the Gulf of Mexico (for Domains 2 and 3). We believe that the relative coarseness of the SST data over the Pacific Ocean or the Atlantic Ocean in this study would not affect the model predictions over the Gulf of Mexico.

2.2 SST Data Processing

In this section, we present the details of the approach we took in arriving at the final SST dataset.

The MODIS SST data was chosen for daily processing. Data from the MODIS instrument is applied in deriving a variety of ocean products. Advanced Very High Resolution Radiometer (AVHRR) has been used in the past to estimate bulk sea temperature. MODIS improves on the capabilities of AVHRR in that ocean color can also be estimated from MODIS measurements. More details about the satellite, instrument and theoretical basis of calculation of SST are available at (http://modis-ocean.gsfc.nasa.gov/refs.html).

The MODIS Level 3 Mapped data was used for our compilation. This data collection has 4.63 and 36 km spatial bins for the entire globe. Henceforth we will refer to the datasets as 4K (4.63 km) and 36K (36 km). The data is presented in a cylindrical equidistant map projection. In total, for 4K (36K) there exist 4096 (512) data grids in the meridional direction and 8192 (1024) grids in the zonal direction corresponding to approximately 4.63 (36) km at the equator. The data is available twice daily: one for the ascending and the other descending path of the satellite in its polar orbit. Moreover, the MODIS team has also processed the data to be output weekly. Each data file has a quality file associated with it. The data and the quality files are combined for a chosen level of quality (best, good, fair or poor) to obtain the final SST values.

As is common with almost all sun-synchronous polar orbiting satellites, on a given day there exist significant gaps in the measured data over the tropics resulting from the orbital path. Moreover, the satellite cannot take measurements below thick clouds. Hence a large number of missing data points also exist over cloudy areas. One such area is Indonesia where thick cumulus clouds exist almost throughout the year.

In the following paragraphs, we discuss the compilation of a contiguous SST dataset with grid spacings of 36 and 4 km starting with the MODIS 36 and 4 km data, respectively.

Owing to the high thermal capacity of water, the diurnal cycle in the temperature of sea water at a given location is typically small. Over short time periods, it is generally reasonable to assume that there would be little variation in the sea surface temperature at a particular grid point.

In arriving at the final SST for a particular day, we took into consideration the SST data for the three days prior and after the day in question. Hence we used up to a total of seven days of data in our calculation. Starting at the end (third day before and third day after) and approaching the current day, the global SST data was superimposed on top of each other. This can be represented by:

$SST_i = SST_i$ or SST_{i+1} or SST_{i-1} or SST_{i+2} or SST_{i-2} or SST_{i+3} or SST_{i-3} — **Step 1**

Where, i is the day for which the data has to be compiled. In the above equation, the global data array is filled from right to left and hence there is an increasing importance of the more recent values than the more distant ones. For example, if the SST data for Day_i at a particular grid point is missing, the value for Day_{i-1} will be used as a replacement if available, otherwise, data for Day_{i+1} is used, etc.

After Step 1, the data gaps arising from the orbital path of the satellite are mostly eliminated. However gaps still exist over areas of thick clouds. As mentioned earlier, persistent clouds can prevent the measurement of SST for more than a week. Hence these gaps in the SST data are still not filled after Step 1.

For the 36K dataset, most gaps are filled after Step 1. However any remaining gaps are filled in Step 3. Hence for this dataset, we jump directly to Step 3 and subsequent processing. The following description for Step 2 involves on the 4K dataset.

The second step (Step 2) involves filling up the remaining gaps with the 36 km SST data. Owing to its coarser resolution, there are fewer spatial gaps in the 36 km data. However, the underlying retrieval algorithm is similar for both the 36 km and the 4 km datasets. Moreover, the 36 km data comprises of a spatial average of approximately 81 adjacent 4 km data cells. Hence any gaps in the 4 km data would be substantially reduced in the 36 km dataset.

Thus,

$SST_i = SST_i$ or $(SST_i)_{36\ km}$ or $(SST_{i+1})_{36\ km}$ or $(SST_{i-1})_{36\ km}$ or $(SST_{i+2})_{36\ km}$ or $(SST_{i-2})_{36\ km}$ or $(SST_{i+3})_{36\ km}$ or $(SST_{i-3})_{36\ km}$ — **Step 2**

Where, SST_i is the 4 km SST value, and the 36 km values are as labeled.

As noted in Table 1, MODIS SST data is available daily as well as weekly. The weekly data is an average of the daily data over the period of interest. Weekly data has most of the data gaps eliminated except for regions with thick cumulus clouds. After Step 2, we fill any remaining gaps with weekly data that may be available. After Steps 1 and 2, if any gaps still exist in the data, filling by the weekly data are expected to be inconsequential. However, our compilation of SST from Steps 1 and 2 and that obtained from the MODIS team may differ slightly. Thus to be on the safer side, we fill the SST data from Step 1 with the MODIS weekly data obtained from the MODIS website.

Thus,

$$SST_i = SST_i \text{ (from Step 2) or } SST_{wi}$$ — **Step 3**

Where, i is for the current day and wi is the week closest to the current day i.

The final step (Step 4) in obtaining a complete 4 km dataset is to fill the remaining gaps – mostly over land and the land-sea boundary. In this case, in order to obtain values at grid cells of missing data, we interpolate data from neighboring grid cells lying under a given radius of influence. In our calculations, we used a 20-grid cell radius of influence. It should be noted that the SST values over land do not exist. However to ingest this dataset in a prognostic model like MM5, a contiguous dataset should be available. The preprocessing steps in MM5 introduce a land-sea mask to eliminate values over land.

The final compiled product is converted into a GRIB format (WMO), using the gribw software (http://wesley.wwb.noaa.gov/gribw.html). The GRIB format is used worldwide in many applications and is compatible with the preprocessing software used in MM5 modeling. The 4K dataset resolution obtained after the MODIS SST compilation is ~ $0.043845^o \times 0.043845^o$. The GRIB format can hold information about the spatial resolution in millilatitudes (10^{-3}) and millilongitudes. Creating a GRIB file at the native resolution would truncate the spatial resolution to $0.043^o \times 0.043^o$. Hence the spatial resolution in the 4K GRIB file was converted to $0.05^o \times 0.05^o$. We do not believe this would affect the spatial distribution of SST. The 36K grib files were left unchanged.

Table 1. Sources and Resolution of Currently Available SST Data

No.	Source	Spatial Resolution	Temporal Resolution	Methodology	Website
1	Final Analysis Data (FNL)	$1^o \times 1^o$	00, 06, 12, 18 Z	Data assimilation	NCEP Tropospheric Analysis http://dss.ucar.edu/datasets/ds083.2/
2	Real-time, global, sea surface temperature analysis (RTG_SST)	$0.5^o \times 0.5^o$	Daily	Analysis of satellite measurements, surface observations and subsequent interpolation	http://polar.ncep.noaa.gov/sst/Welcome.html
3	AVHRR Pathfinder Data	9, 18, 54 km	Daily, weekly, monthly	Satellite measurements	http://podaac.jpl.nasa.gov/sst
4	AVHRR Multi-channel SST (MCSST)	18 km	Weekly	Satellite measurements	http://podaac.jpl.nasa.gov/mcsst
5	MODIS SST	4 km	Daily, weekly	Satellite measurements	http://modis-ocean.gsfc.nasa.gov/
6	NAVOCEANO MCSST	9 km	Daily	Satellite measurements	http://podaac.jpl.nasa.gov/navoceano_mcsst
7	NCEP Reynolds Optimally Interpolated (OI) SST	$1^o \times 1^o$	Weekly, monthly	Satellite measurements	
8	Along-Track Scanning Radiometer (ATSR)	1 km		Satellite measurements	http://www.atsr.rl.ac.uk/atsr/index.shtml

3. RESULTS

3.1 SST over the United States.

Our compilation of the 36K data for the whole United States is presented in Figure 2 (2a through 2d). For comparison, we employed the NCEP Reynolds OI SST data (Source 7 in Table 1) [Reynolds and Smith, 1994] and the Real Time Global SST data (Source 2 in Table 1) [Thiébaux et al., 2001]. Our compilation of the MODIS SST and the RTG SST was available daily, while the Reynolds SST was available weekly. Moreover, the RTG SST data compilation started in February 2001. Hence comparison of MODIS SST prior to February 2001 was done only with the Reynolds SST.

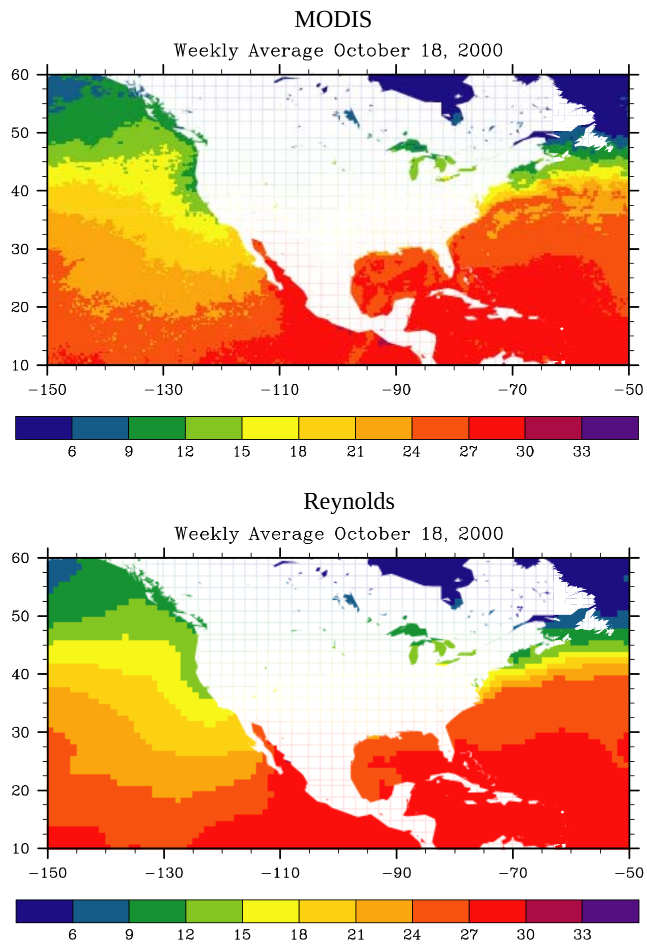


Figure 2a.

Figure 2. Horizontal plot of SST values over the Gulf of Mexico (units = °C). (a) October 18, 2000, (b) January 17, 2001, (c) April 18, 2001, and (d) July 18, 2001. The weekly MODIS and RTG data is obtained by averaging seven days of daily data that include three days before and after the day of interest. Spatial resolutions of MODIS, Reynolds and RTG SST data are 0.35×0.35, 1×1, and 0.5×0.5 degrees, respectively.

In Figure 2, weekly average values for MODIS SST are shown for October 18, 2000, January 17, 2001, April 18, 2001, and July 18, 2001. The weekly averages were calculated from the daily values three days before and after the day in question, for a total of seven days. Similar approach was taken for the RTG SST data that is available daily.

As seen in Figure 2a, large-scale features in the SST values are captured in both the MODIS and the Reynolds SST data. For example, warmer Gulf Stream temperatures (24-27 ^{o}C) extending from North Carolina to the mid Atlantic Ocean are seen in both data. The coarseness of the Reynolds data is clearly visible in the bottom plot. This coarse resolution is also responsible for the lack of colder waters (9-12 ^{o}C) along the western coast of the United States, which are seen in the MODIS data. Another interesting feature observed in the MODIS data that is not visible in the Reynolds data is the colder water temperatures in Lake Superior. Although, this feature is not relevant to the present study, such differences in two datasets are important in future work where modeling near coastal regions need to be done.

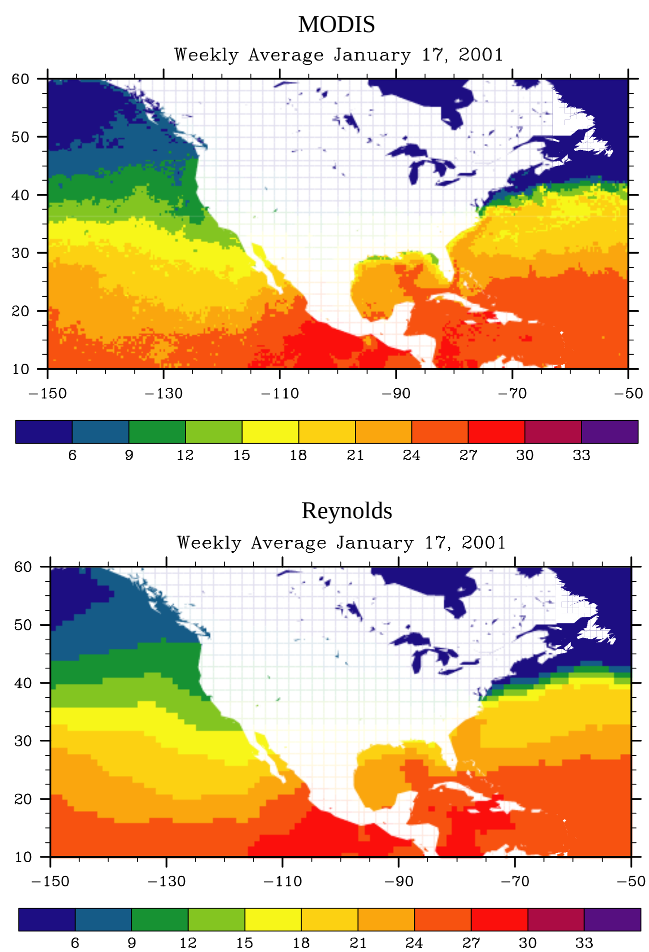


Figure 2b.

In January, colder water temperatures are seen along the US Gulf coast in the MODIS SST. This feature is absent in the Reynolds dataset. In April, a small eddy feature off the Eastern US is seen in both the MODIS and RTG, but not in the Reynolds. Finer resolution of the MODIS and RTG datasets thus has the capability of capturing such small-scale features in ocean temperatures. Finally, in July, colder water temperatures off the coast of California are seen in all three datasets. However, the MODIS data exhibits greater details than the other two datasets.

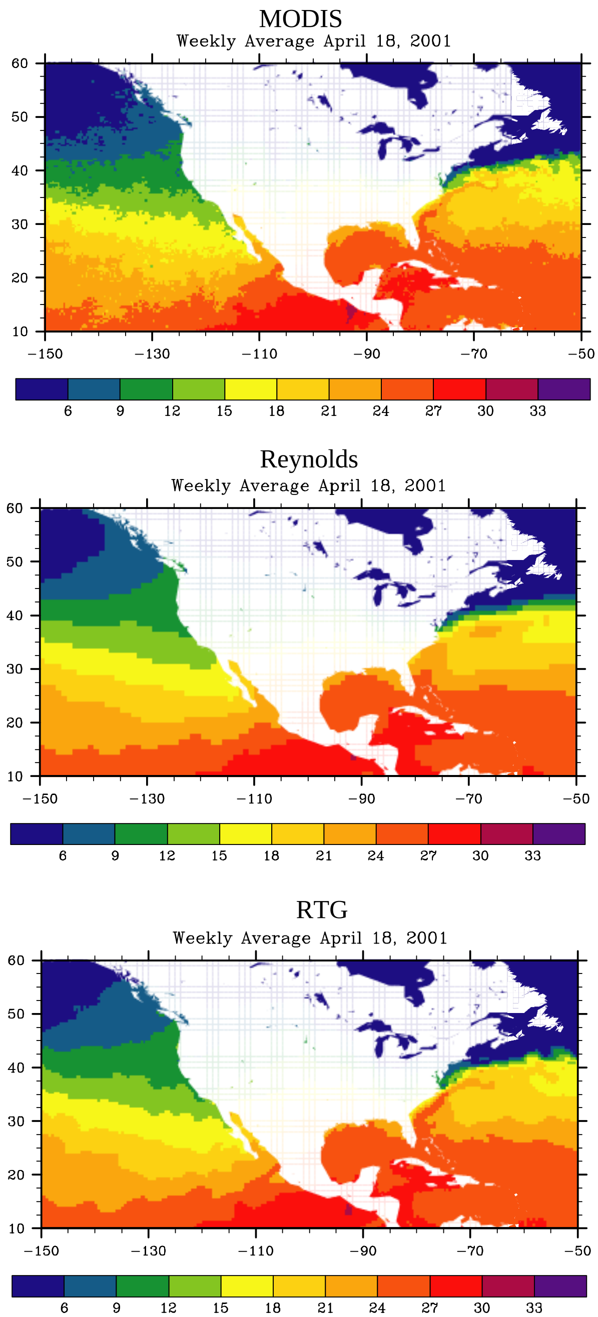


Figure 2c.

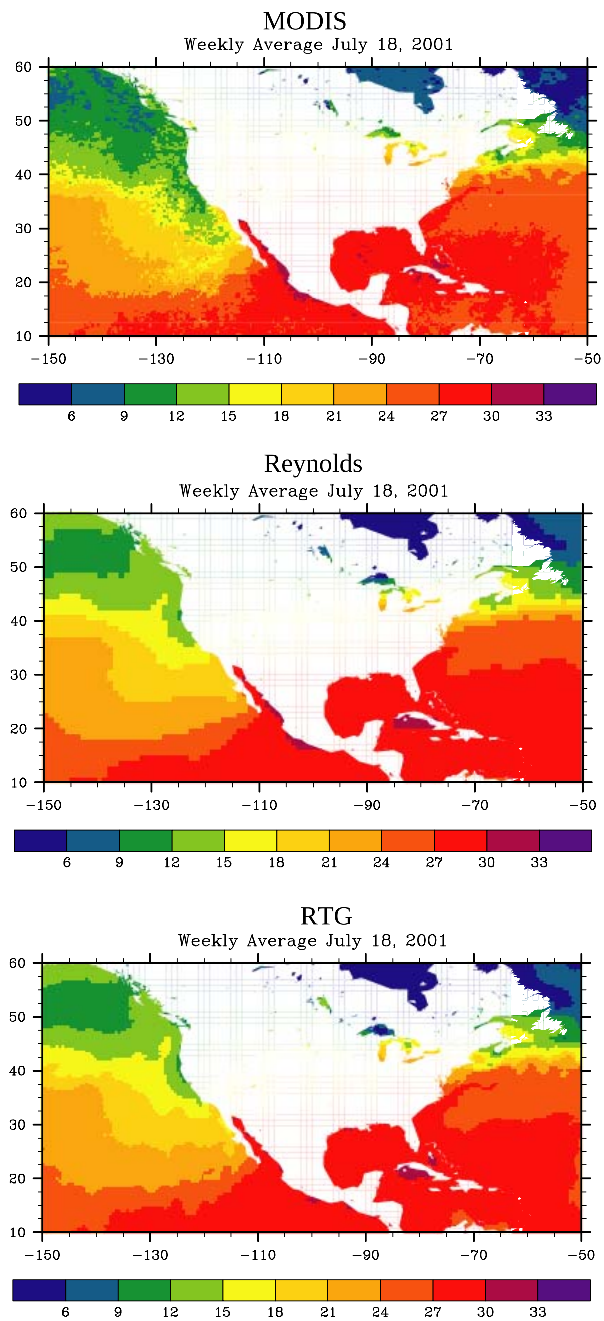


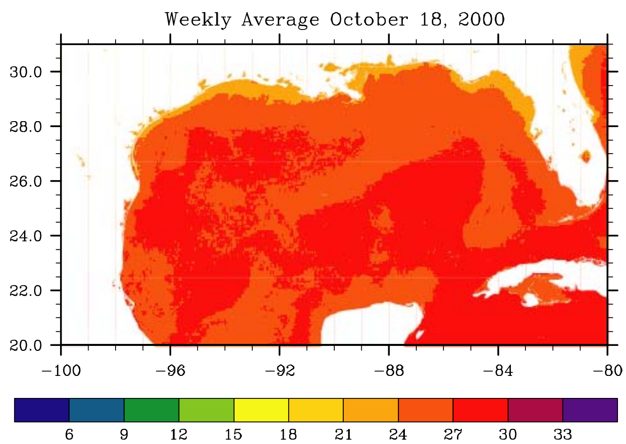
Figure 2d.

3.2 SST Over the Gulf of Mexico

Domains 2 and 3 in MM5 modeling are located over the Gulf of Mexico. Therefore, we examined the SST data in detail over the Gulf of Mexico. We used the 4K data for this purpose. This analysis is presented in Figure 3 (3a through 3d) and is similar to the one presented in Figure 2.

As seen in Figure 3, the MODIS SST values for October 18, 2000 are more or less comparable to the Reynolds SST values. Warm water temperatures (27-30°C) are evident closer to the tropics and south and east of Key West. These warm temperatures also extend in the middle of the Gulf of Mexico. The MODIS SST data exhibits peculiar features not observed in the Reynolds data. For example, the water temperatures in the proximity of coastal United States tend to be lower in the MODIS SST than the Reynolds SST dataset. While the average water temperature near the southern coast of the United States from the Reynolds SST is between 24 and 27°C, those values from the MODIS SST data tend to be between 21 and 24°C. This difference can be attributed to the relative coarseness of the Reynolds SST data.

MODIS



Reynolds

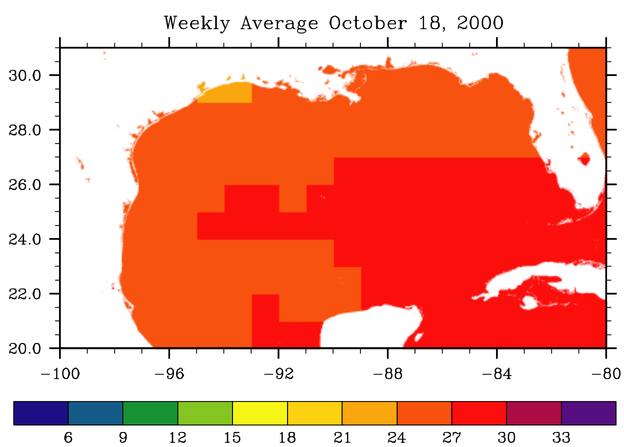
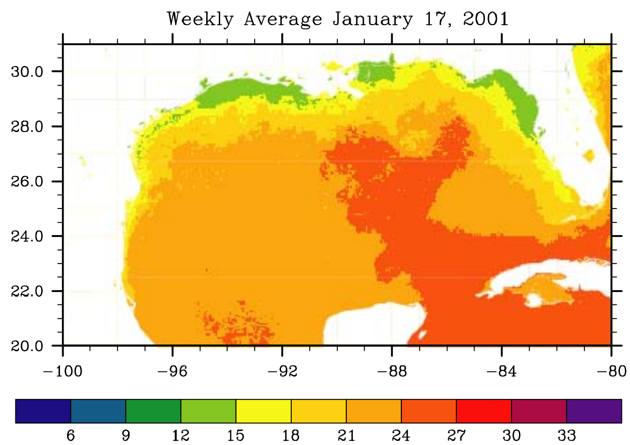


Figure 3a.

Figure 3. Horizontal plot of SST values over the Gulf of Mexico (units = °C). (a) October 18, 2000, (b) January 17, 2001, (c) April 18, 2001, and (d) July 18, 2001. The weekly MODIS and RTG data is obtained by averaging seven days of daily data that include three days before and after the day of interest. Spatial resolutions of MODIS, Reynolds and RTG SST data are 0.05 × 0.05, 1 × 1, and 0.5 × 0.5 degrees, respectively.

Similar features are also observed in the January 17, 2001 comparison. While the open ocean temperatures of 24-27^{o}C are comparable in both datasets, the coastal values from MODIS tend to be biased lower. Also, an unique feature observed in the MODIS data is the isolated maxima/minima over the shallow waters south of northwest Cuba. The colder water temperature along the coastal United States could also be a result of the ocean depth. This needs to be investigated in the future.

MODIS



Reynolds

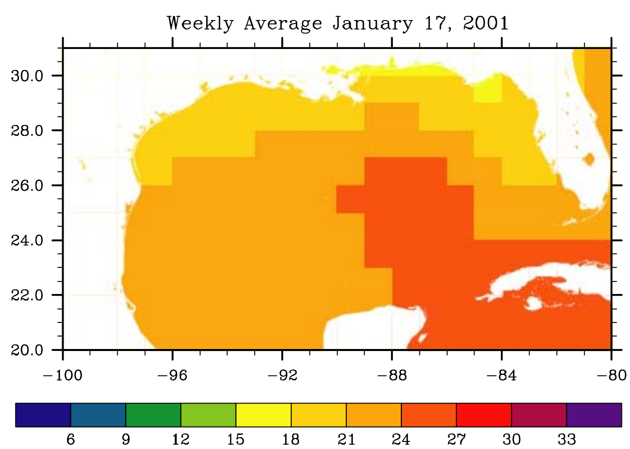
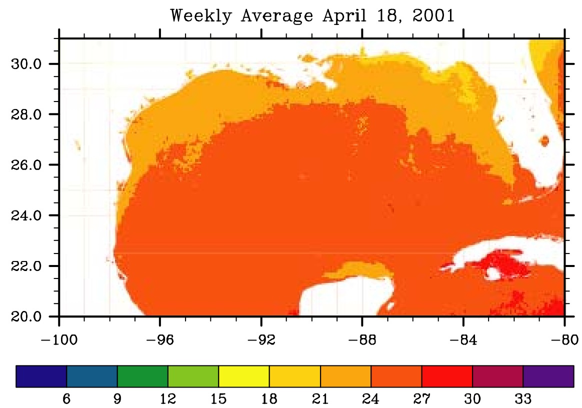
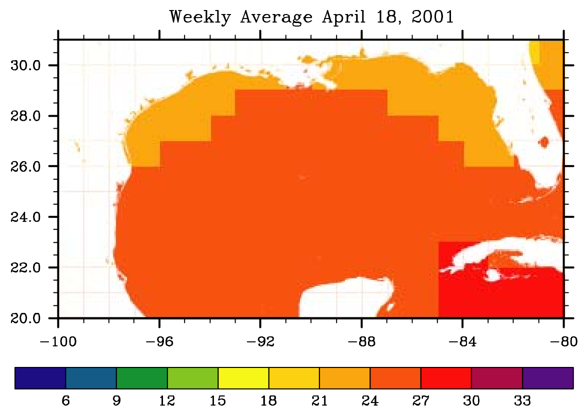


Figure 3b.

MODIS



Reynolds



RTG

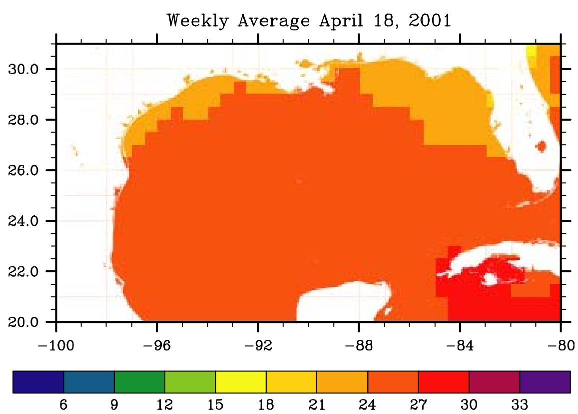


Figure 3c.

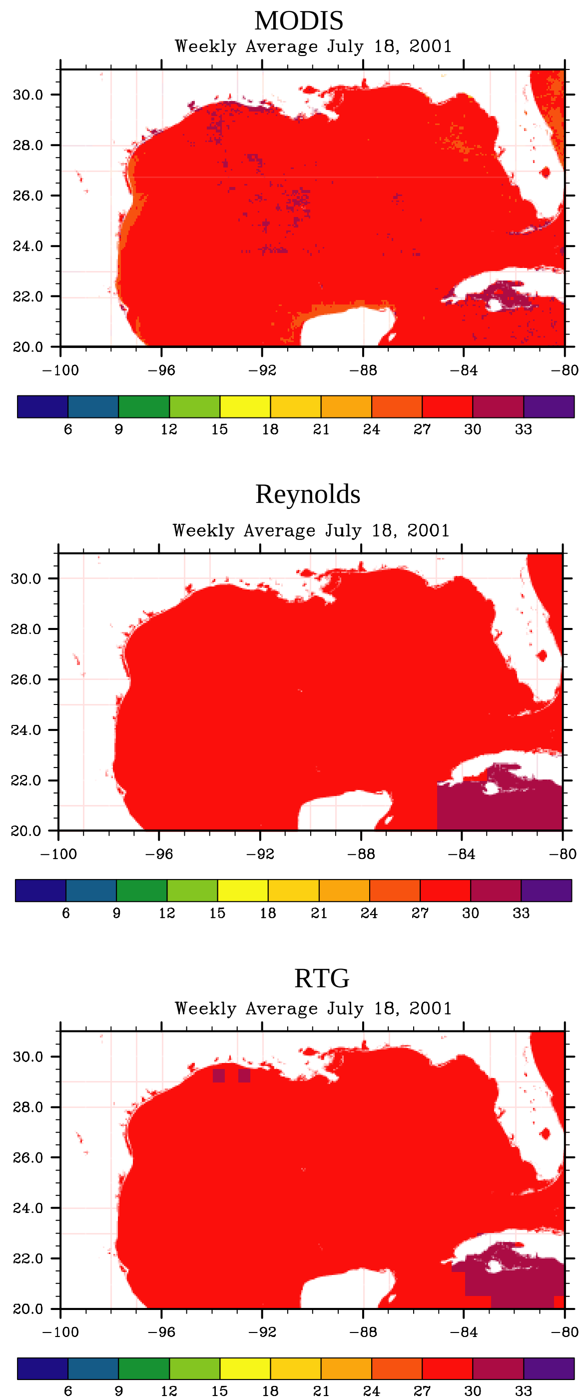

MODIS
Weekly Average July 18, 2001
30.0
28.0
26.0
24.0
22.0
20.0
−100
−96
−92
−88
−84
−80
6 9 12 15 18 21 24 27 30 33
Reynolds
Weekly Average July 18, 2001
30.0
28.0
26.0
24.0
22.0
20.0
−100
−96
−92
−88
−84
−80
6 9 12 15 18 21 24 27 30 33
RTG
Weekly Average July 18, 2001
30.0
28.0
26.0
24.0
22.0
20.0
−100
−96
−92
−88
−84
−80
6 9 12 15 18 21 24 27 30 33

Figure 3d.

3.3 Comparison with Data from Other Sources

Further validation of the SST data from MODIS was done by comparisons with surface based observations. Hourly ocean buoy data over the Gulf of Mexico is available from the National Data Buoy Center (http://www.ndbc.noaa.gov). Data over the Gulf of Mexico was extracted from the observed data and plotted against that derived from our compilations. The locations of the buoys are shown in Figure 4 and Table 2. This evaluation is presented in Figure 5 (a through j). The hourly ocean buoy data at these locations was averaged to a daily value and plotted against the daily values from the MODIS dataset. The data used in the analysis was for a time period October 2000 to September 2001. Since the MODIS data was only partly available for June and July 2001, SST values during these two months were not included in our analysis. Also, missing days from the buoy data along with corresponding days in the MODIS data were also omitted from the analysis.

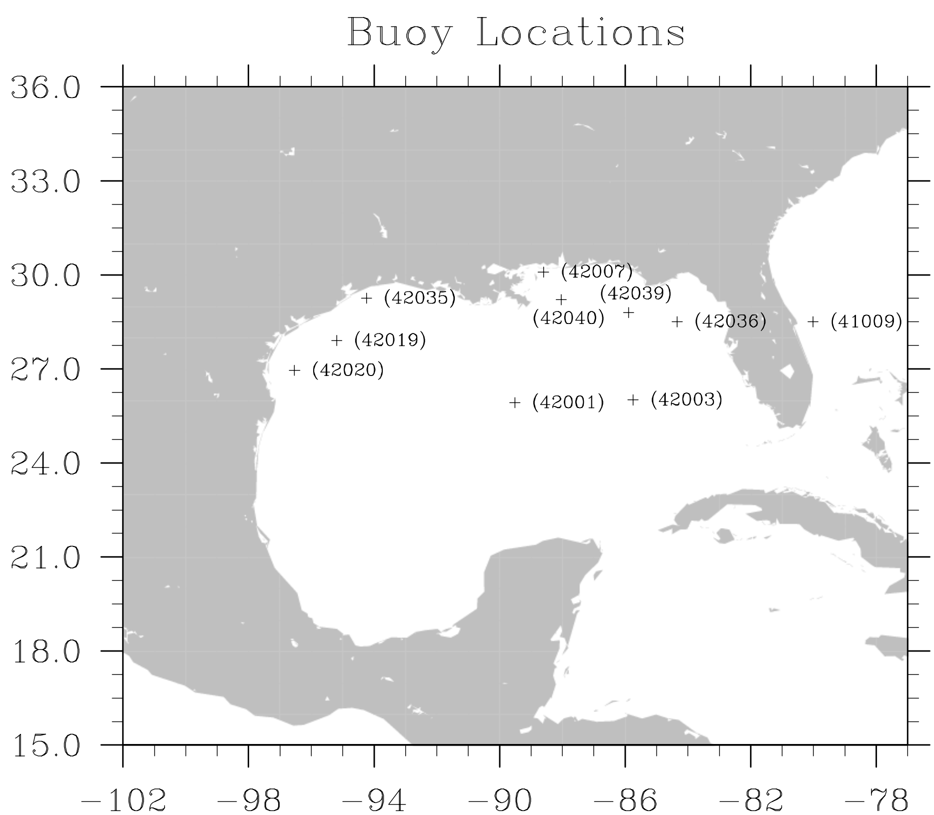


Figure 4. Locations of the stations from which the buoy SST data was obtained. The '+' sign gives the geographic location, while the number in the parenthesis is the station number. Note that most of the stations are located near the United States only.

From Table 2 and Figure 5, it can be seen that the satellite-derived SST values are in very good comparison with the observed SST from buoys. Cross correlation coefficients between the MODIS and buoy SST values exceed 0.9 for all stations except Galveston. This represents an excellent match between what is calculated by the MODIS algorithms and that observed at the ocean surface. The relatively lower correlation between the two SST data at Galveston is unknown and needs to be studied more.

Table 2. Correlation Coefficients MODIS Data Versus Buoy Data

Station Number	Station Name	Latitude (N)	Longitude (W)	Number of Points	Correlation Coefficient
41009	Canaveral West	28.5	80.18	302	0.958
42001	Mid Gulf	25.92	89.68	304	0.967
42003	E Gulf	26.01	85.91	304	0.957
42007	Biloxi	30.09	88.77	304	0.992
42019	Freeport	27.91	95.36	304	0.940
42020	Corpus Christi	26.95	96.7	276	0.962
42035	Galveston	29.25	94.41	248	0.828
42036	West Tampa	28.51	84.51	304	0.991
42039	Pensacola	28.8	86.06	268	0.982
42040	Mobile South	29.21	88.20	292	0.971

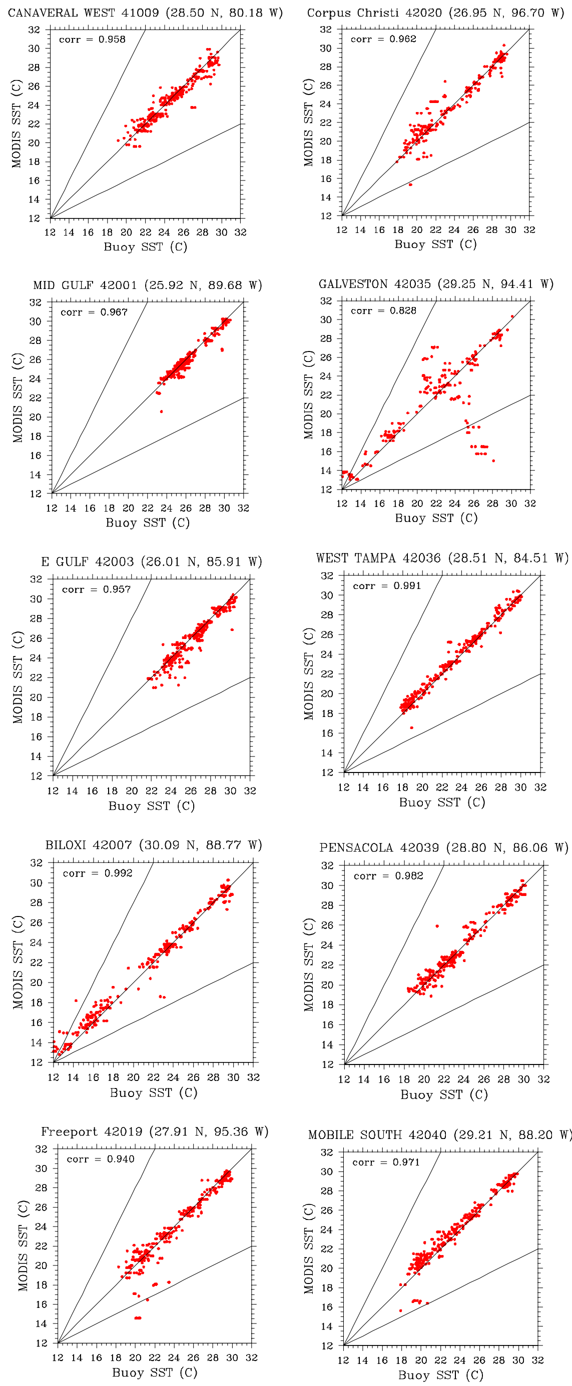


Figure 5. Comparison between MODIS and buoy SST values. The points represent data for a period of one year (October 2000 – September 2001, except June – July 2001). Missing data in buoy observations are removed. Days corresponding to the missing buoy data days are also removed from the MODIS data. Also shown in the plots are 1:1, 1:2 and 2:1 lines. The name and location of the station is shown above each plot.

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