Improving the Accuracy of Satellite Sea Surface Temperature Measurements by Explicitly Accounting for the Bulk-Skin Temperature Difference

Final Report, NASA Grant NAG5-10288

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Abstract

The focus of this research was to determine whether the accuracy of satellite measurements of sea surface temperature (SST) could be improved by explicitly accounting for the complex temperature gradients at the surface of the ocean associated with the cool skin and diurnal warm layers. To achieve this goal, work centered on the development and deployment of low-cost infrared radiometers to enable the direct validation of satellite measurements of skin temperature. During this one year grant, design and construction of an improved infrared radiometer was completed and testing was initiated. In addition, development of an improved parametric model for the bulk-skin temperature difference was completed using data from the previous version of the radiometer. This model will comprise a key component of an improved procedure for estimating the bulk SST from satellites. The results comprised a significant portion of the Ph.D. thesis completed by one graduate student and they are currently being converted into a journal publication.

Introduction

The presence of the cool skin and diurnal warming of the oceanic near-surface layer create a source of uncertainty in efforts to retrieve the bulk SST using satellite data. While the bulk SST is typically representative of temperatures at near 1 m in depth, infrared satellite sensors measure only the radiation emitted from the upper ~10 microns of the ocean surface. The cool skin and warm layer lead to significant and highly variable differences between these skin and bulk temperatures. Traditional operational bulk SST algorithms (e.g. May et al., 1998) have just directly regressed the satellite brightness temperature measurements of the skin layer against in situ measurements of the bulk SST from buoys and ships. The potential for improving the accuracy of satellite SST measurements by explicitly treating these cool-skin and warm-layer effects motivated the research performed under this project.

The primary path of this research centered on attempting to increase the number of in situ observations of the oceanic skin temperature from ships to enable better direct validation of satellite skin measurements and production of a satellite skin SST product. A second related course of research focused on developing improved models of the warm layer and cool skin so that bulk and skin SST measurements could be better related and the skin effect explicitly included in satellite SST retrievals.

This project represented a one-year extension of NASA Grant NAG5-6521 of the same name. The extension was required in order to enable the completion of an improved seagoing infrared radiometer. A first radiometer was constructed and deployed under the initial grant, but the deployments demonstrated that this radiometer was not robust enough to work reliably over long periods at sea. The additional year also enabled the completion of the Ph.D. thesis of Sandra Castro (Castro, 2001) who applied the data from the first radiometer to the development of an improved parametric model of the skin layer. A final report for the initial grant was submitted this February and included a description of some of the activities during the year extension along with a summary of the overall project. A copy of the report for NAG5-6521 is included at the end of this report as appendix A for reference. The remainder of this report will focus in more detail on the specific activities in the one year covered by NAG5-10288.

Development of a Ship-of-Opportunity Radiometer

The goal of the radiometer development was to produce a low-cost infrared radiometer that could be deployed in large numbers on ships of opportunity where little operator intervention is available. The need for many radiometers arises from the requirement for large numbers of matches with clear-sky satellite observations to sufficiently validate satellite SST products. When deployed in large numbers, the radiometers must be capable of performing reliably over long periods with little maintenance from the operators. Providing, robustness, a low cost, and an accuracy sufficient for meaningful validation (0.1 K targeted) was a very difficult development challenge.

An initial radiometer named the Ship of Opportunity Sea Surface Temperature Radiometer or SOSSTR was developed and deployed under the initial funding of this project. Multiple deployments of the SOSSTR illustrated that while the instrument was capable of producing scientifically useful data, it was not robust enough to function autonomously at sea for long durations. Development of a second radiometer system was begun by Dr. Joe Shaw and Hector Bravo of the NOAA Environmental Technology Laboratory (ETL). An initial design attempted to avoid use of a chopper wheel and directly obtain differential measurements between the sea, sky, and blackbodies. Testing revealed, however, that the detectors could not settle rapidly enough and that a different design would be required. At this point, however, the initial funding had expired and the one-year extension was required.

During the one year extension, the ETL group refined the design of the radiometer and constructed a prototype system. The final design utilized directly purchased infrared detectors, off-the-shelf filters, and relatively low cost commercial blackbodies. One blackbody included a temperature control system so that it could be maintained roughly 5 K above the local SST. The other blackbody was allowed to float at the ambient temperature and simply contained a system to accurately monitor its temperature. A rotating mirror assembly to sequentially view the blackbodies, sea and sky was locally fabricated along with a chopper wheel system. All data logging and instrument control functions were performed using available computers and new software developed in the Labview environment. The total hardware cost for the new radiometer was kept below $25,000. The most significant cost savings were achieved through the use of individual detectors and filters rather than a commercial package. Two photographs of the prototype radiometer are shown in Figure 1.

The radiometer was tested in a laboratory at ETL using additional blackbodies to simulate the sea and sky temperatures. The tests demonstrated that the design performed as expected and that an accuracy approaching 0.1 K would likely be possible at least in the laboratory. This system is currently being readied for an extended rooftop test to more fully test its radiometric performance and evaluate its ability to operate autonomously while exposed to the environment.

Only some minor modifications to the radiometer design are still required. A small watertight door that is triggered by a rain sensor must still be fabricated and attached to the system. This system will allow the radiometer to seal itself in the case of rain or excessive spray. The other modifications consist of some minor software additions and changes. If the rooftop test is successful, the radiometer system will be deployed to sea at the first available opportunity.

Refinement of Models for the Cool Skin

The one-year extension also helped to fund the completion of the Ph.D. thesis of Dr. Sandra Castro (Castro, 2001). The focus of this work was to develop a refined model for the bulk-skin temperature difference that could better reproduce observed variability under a diverse range of environmental conditions. This model can now be applied to new satellite retrievals of the bulk SST that attempt to explicitly account for the skin effect. An example of this technique is shown in the work of Wick et al. (2002) that was performed as part of the initial funding of this project. The model improvements of Castro (2001) should be key in bettering the preliminary results found by Wick et al.

The work of Castro resulted in a new surface renewal type model for the temperature change across the nighttime skin layer in which the combined effects of simultaneous physical processes are accounted for through a weighted sum of the individual contributing mechanisms. Each mechanism is treated using a unique surface renewal time scale. Four new time scales were developed to account for mechanisms that had not been previously considered in skin layer models. These mechanisms included a shear saturation regime, capillary waves, microscale breaking, and large-scale breaking. These new time scales were then combined with existing time scales for free convection and wind shear processes. A classification scheme was developed to determine weights indicating the relative importance of each mechanism. The weights were found to be functions of the net heat flux, observed temperature and the Richardson and Rayleigh numbers and are computed independently at each data point. Once the weights are determined, the bulk-skin temperature difference is computed through a linear combination of the temperature difference resulting from each mechanism given by:

$$\Delta T = W_{conv}\Delta T_{r,conv} + W_{shear}\,\Delta T_{r,shear} + W_{shearsat}\,\Delta T_{r,shearsat} + W_{capil}\,\Delta T_{r,capil} + W_{\mu sb}\,\Delta T_{r,\mu sb} + W_{lsb}\,\Delta T_{r,lsb}.$$

A complete definition of all the time scales and classification scheme is included in Castro (2001).

The new model was found to provide a significant improvement over previous parameterizations and seems to capture the relevant physics of small-scale processes and their effect on the bulk-skin temperature difference. An illustration of the performance of the model applied to two independent data sets is shown in Figure 2. The model is found to reproduce the observations with very high correlation and low rms errors. The accuracy and predictability of the model offer additional support for the relevance of the physical mechanisms on which it is based and substantiate the newly derived time scales used in the model. Dr. Castro is currently completing a journal publication based on these results.

Conclusions

Through two different paths of research undertaken as part of this project, significant progress was made towards improving the accuracy of satellite SST retrievals by explicitly accounting for the complex temperature gradients at the surface of the ocean associated with the cool skin and diurnal warm layers. To conclude, we include a list of the most significant accomplishments:

- Design and fabrication of an improved low-cost infrared radiometer system for collecting large numbers of in situ observations of the radiometric skin temperature of the ocean from ships of opportunity was completed.
- Initial laboratory testing of the radiometer was completed and preparations are being made for an extended rooftop test.
- A significantly improved model for the temperature difference across the cool skin was developed using data from a previous version of the radiometer developed under initial funding.
- Dr. Sandra Castro was able to complete her Ph.D. dissertation and is now completing a manuscript for journal publication based on these results.

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Wick, G. A., J. J. Bates, and D. J. Scott, 2001: Satellite and skin layer effects on the accuracy of sea surface temperature measurements from the GOES satellites. *J. Atmos. Ocean. Technol.*, submitted.

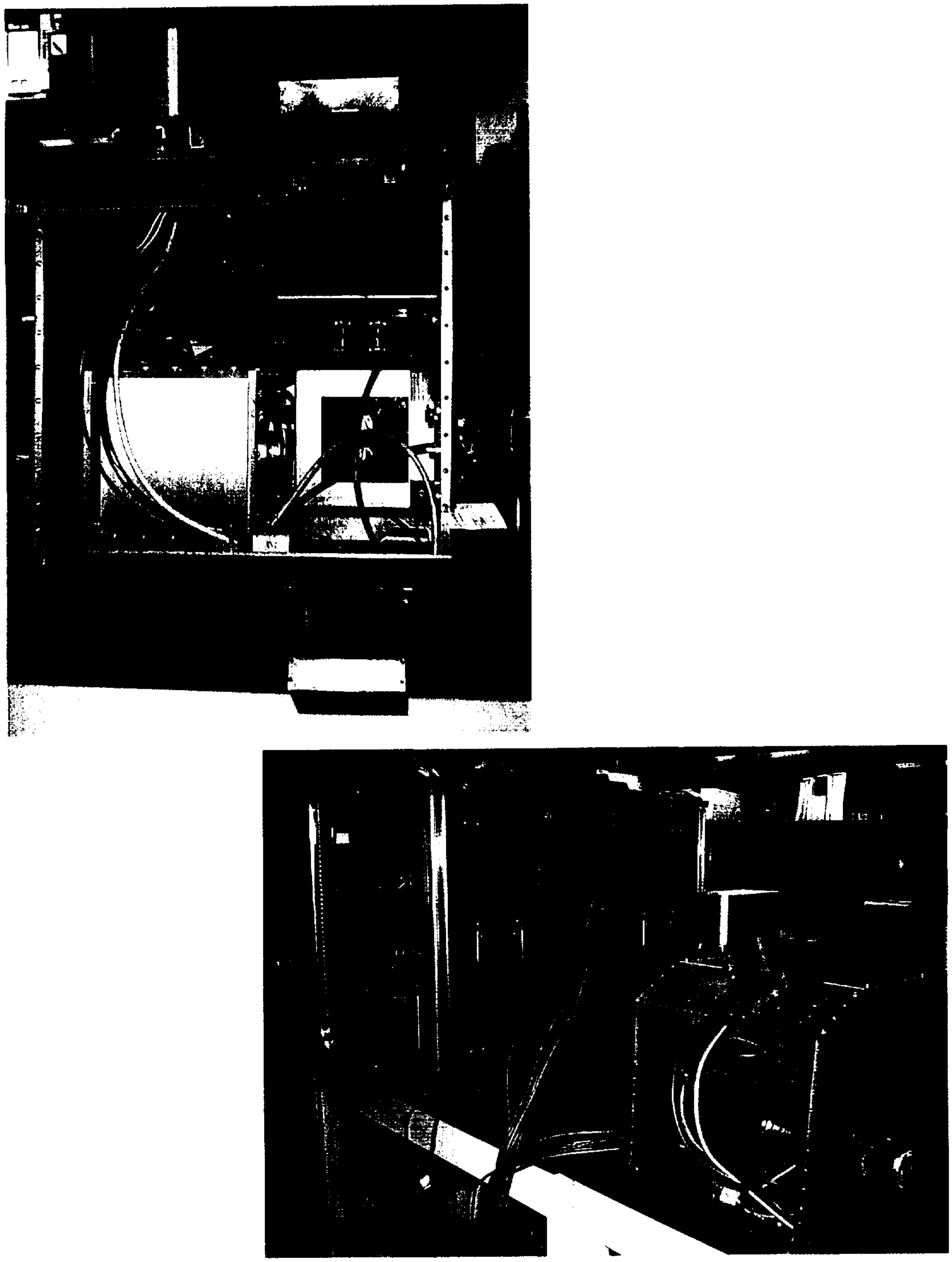
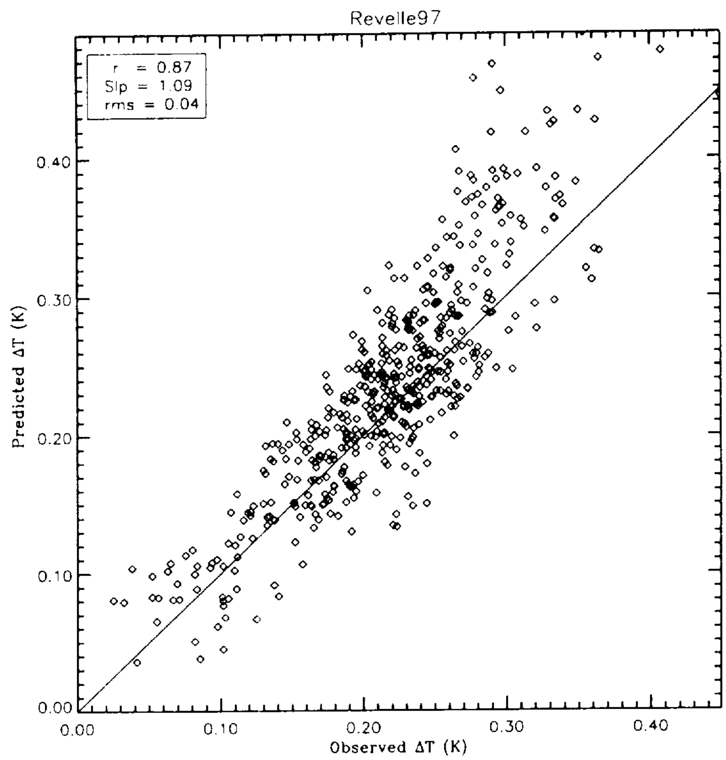


Figure 1. Photographs of the radiometer system designed and constructed through this project. The upper panel shows a view into the radiometer head assembly showing the radiometer lens, blackbodies, and upward and downward looking viewing ports. Note that the scanning mirror has been removed in this photograph. The lower panel shows the head assembly along its accompanying electronics box. The box houses the logging computer and blackbody control mechanism. The motor seen on the outside of the head assembly drives the scanning mirror.



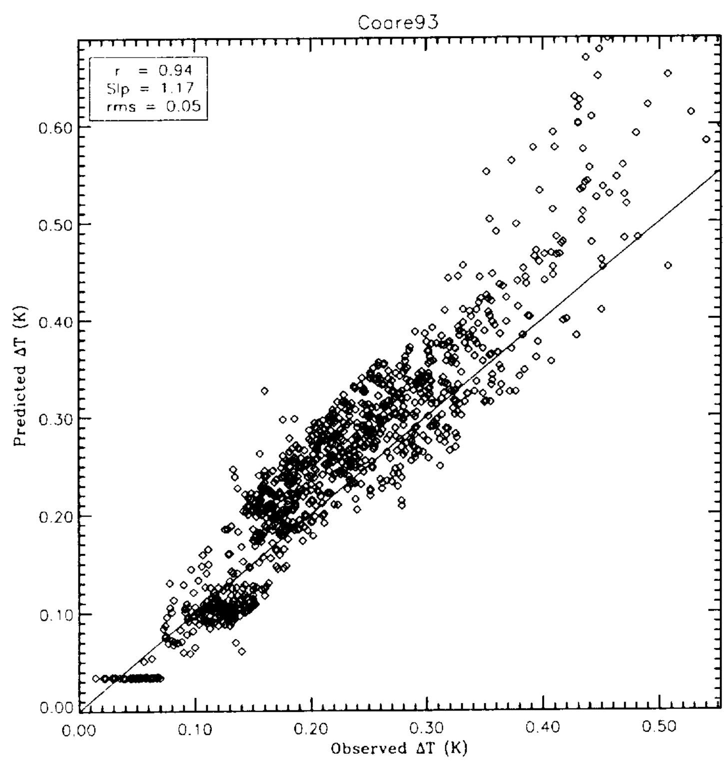


Figure 2. Evaluation of the new skin layer model against direct observations from two independent cruises not used in the development of the model.

Appendix A.

Improving the Accuracy of Satellite Sea Surface Temperature Measurements by Explicitly Accounting for the Bulk-Skin Temperature Difference

Final Report, NASA Grant NAG5-6521

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February, 2002

Abstract

The focus of this research was to determine whether the accuracy of satellite measurements of sea surface temperature (SST) could be improved by explicitly accounting for the complex temperature gradients at the surface of the ocean associated with the cool skin and diurnal warm layers. To achieve this goal, work was performed in two different major areas. The first centered on the development and deployment of low-cost infrared radiometers to enable the direct validation of satellite measurements of skin temperature. The second involved a modeling and data analysis effort whereby modeled near-surface temperature profiles were integrated into the retrieval of bulk SST estimates from existing satellite data. Under the first work area, two different seagoing infrared radiometers were designed and fabricated and the first of these was deployed on research ships during two major experiments. Analyses of these data contributed significantly to the Ph.D. thesis of one graduate student and these results are currently being converted into a journal publication. The results of the second portion of work demonstrated that, with presently available models and heat flux estimates, accuracy improvements in SST retrievals associated with better physical treatment of the near-surface layer were partially balanced by uncertainties in the models and extra required input data. While no significant accuracy improvement was observed in this experiment, the results are very encouraging for future applications where improved models and coincident environmental data will be available. These results are included in a manuscript undergoing final review with the Journal of Atmospheric and Oceanic Technology.

Introduction

The presence of the cool skin and diurnal warming of the oceanic near-surface layer create a source of uncertainty in efforts to retrieve the bulk SST using satellite data. While the bulk SST is typically representative of temperatures at near 1 m in depth, infrared satellite sensors measure only the radiation emitted from the upper ~10 microns of the ocean surface. The cool skin and warm layer lead to significant and highly variable differences between these skin and bulk temperatures. Traditional operational bulk SST algorithms (e.g. May et al., 1998) have simply directly regressed the satellite brightness temperature measurements of the skin layer against in situ measurements of the bulk SST from buoys and ships. The potential for improving the accuracy of satellite SST measurements by explicitly treating these cool-skin and warm-layer effects motivated the research performed under this project.

Two different but related paths of research were undertaken to explore possible accuracy improvements. The first path centered on attempting to increase the number of in situ observations of the oceanic skin temperature from ships to enable better direct validation of satellite skin measurements and production of a satellite skin SST product. The long-term goal of this work was to determine if an adequately validated satellite skin SST product could be shown to have a higher accuracy (in terms of lower RMS error) than traditional bulk SST algorithms. To achieve this goal, two different low-cost infrared radiometers were developed for deployment at sea with minimal operator intervention. The first of these was successfully deployed during two research cruises and the data were used for related scientific research as well as for the refinement of the radiometer design.

The second course of research focused on determining if the accuracy of satellite bulk SST products could be improved by including models of the warm layer and cool skin effects in the retrieval scheme rather than only directly regressing the satellite measurements against observed bulk SST values. An experiment was conducted using GOES data where two algorithms using either direct regression or explicit consideration of the near-surface layer were compared during a common evaluation period. These results are included in a manuscript undergoing final review with the Journal of Atmospheric and Oceanic Technology. More complete details of both these lines of research and their results are included in the remainder of this report.

Development of a Ship-of-Opportunity Radiometer

The first and largest portion of the research under this project involved the development of an infrared radiometer system that could be deployed in large numbers on volunteer observing ships or ships of opportunity. Large numbers of observations are required to enable sufficient validation of a skin SST product. The prevalence of satellite bulk SST algorithms despite the fact that the satellite measurements are actually of skin temperature is due in part to the large number of bulk SST measurements from buoys and ships available for validation. Despite many previous research cruises targeted at research on the skin layer and validation of products from the ATSR and MODIS, still only a relatively small number of matches between clear-sky satellite observations and in situ skin temperature measurements exist. The number of research cruises is simply too small to produce measurements equal in number to the bulk SST measurements available from drifting and moored buoys and various commercial ships. To increase the number of skin temperature measurements, it was necessary to develop a radiometer package that could be easily deployed on ships of opportunity.

The requirement for multiple radiometers dictated a low cost while the need to deploy them with minimal operator intervention required a robust design that prevented the measurements from being compromised by the harsh marine environment. To be useful for satellite validation, a high measurement accuracy of 0.1 K or better was also required. These requirements presented a very difficult development challenge.

The first radiometer developed under this project focused on a very low cost design and was envisioned as a test bed to facilitate the production of a final design. This radiometer was named the Ship of Opportunity Sea Surface Temperature Radiometer or SOSSTR. Development of the SOSSTR was led by Dr. Craig Donlon while working in a post-doctoral position under Dr. William Emery. The design of the SOSSTR was built around two single-channel, broadband (8-12 μm) TASCO THI-500L radiometers. Initial testing suggested that these low-cost commercial radiometers were capable of maintaining a calibration of +/- 0.1 K. The first radiometer was fixed viewing the sea surface. The second viewed the sky at a zenith angle equivalent to the nadir angle of the sea-viewing radiometer to enable correction for sky reflection. Two blackbodies, one at a slightly elevated temperature and the other at ambient, were rotated through the field of view of both radiometers to enable accurate calibration. This entire assembly was enclosed in a rugged box with a small aperture cut for the radiometers to view the sea and the sky. A fan was used to force air out of the aperture in an effort to prevent water ingress and contamination of the radiometer optics. A schematic illustration of the basic components of the SOSSTR is shown in Figure 1. Initial testing and calibration of the SOSSTR was performed at the First Infrared Radiometer Intercomparison held at the University of Miami in March, 1998.

The SOSSTR was deployed on the RRS James Clark Ross in October 1998 by Dr. Craig Donlon during a cruise from England to the Falkland Islands. The instrument operated successfully during the majority of a 28-day period producing simultaneous sea and sky brightness temperature measurements. A sample of the raw measurements collected during one day is shown in Figure 2. The dual spikes apparent regularly in the data correspond to the black body views. A complex software processing package was developed to extract the calibration views and use the corresponding data to calibrate the sea and sky measurements. This processing package was applied to the entire data set to produce a time series of skin temperature corrected for atmospheric reflection effects. Excerpts of this time series are shown along with the corresponding wind speed and net air-sea heat flux in Figure 3. The limited number of data points correspond to the instances where all the instruments required for the SST and flux measurements were functioning and were not influenced by rain or adverse airflow around the ship.

These measurements were incorporated as one of several data sets used in the Ph.D. thesis research of Dr. Sandra Castro (Castro, 2001). Castro used the data to help evaluate and refine models for the cooling across the skin layer during the nighttime. A comparison of the predictions of the model developed by Castro with the corresponding measurements from the SOSSTR and other instrumentation on the RRS James Clark Ross is shown in Figure 4. The model demonstrated similar success in reproducing the observations from several other cruises and radiometer packages. These results help illustrate the scientific merit of the data collected by the SOSSTR. Dr. Castro is currently preparing a journal publication based on the results from her completed dissertation.

The SOSSTR was also deployed during the Gas Exchange Experiment (GasEx) in the North Atlantic in 1998. Analyses of these data were complicated by the failure of a multiplexer in the data logging package but several periods of usable data were collected during this experiment. A detailed scientific analysis of all these data has not yet been completed.

The multiple deployments of the SOSSTR illustrated that while the instrument was capable of producing scientifically useful data, it was not robust enough to function autonomously at sea for long durations. In addition, the TASCO radiometers were found to have some characteristics that prevented them from being the optimum radiometer choice. Development work was therefore begun on a second radiometer. The development was initially delayed by the departure of Dr. Donlon following the completion of his post-doctoral appointment at the University of Colorado. Dr. Joe Shaw and Hector Bravo of the NOAA Environmental Technology Laboratory (ETL) were then contacted and took over the development of the second radiometer.

The ETL group attempted to keep costs down by directly purchasing infrared detectors and off-the-shelf filters rather than designing around a commercially available infrared radiometer. Relatively low cost commercial blackbodies were purchased from Eppley Laboratories. One blackbody included a temperature control system so that it could be maintained roughly 5 K above the local SST. The other blackbody was allowed to float at the ambient temperature and simply contained a system to accurately monitor its temperature. All data logging and instrument control functions were performed using available computers and new software developed in the Labview environment. The total cost for hardware and construction was targeted to be less than $25,000.

An initial design attempted to avoid use of a chopper wheel and directly obtain differential measurements between the sea, sky, and blackbodies. Testing revealed, however, that the detectors could not settle rapidly enough and a second, more traditional design using a chopped signal was adopted. The design change did not significantly change the equipment or construction costs. Using an extension in funding, a complete system was constructed and tested in the laboratory using additional blackbodies to simulate the sea and sky temperatures.

This system is currently being readied for an extended rooftop test to more fully test its radiometric performance and evaluate its ability to operate autonomously while exposed to the environment. Only some minor modifications to the design are still required. A small watertight door that is triggered by a rain sensor must still be fabricated and attached to the system. This system will allow the radiometer to seal itself in the case of rain or excessive spray. The other modifications consist of some minor software additions and changes. If the rooftop test is successful, the radiometer system will be deployed to sea at the first available opportunity.

Explicit Treatment of the Warm Layer and Cool Skin in Bulk SST Retrievals

The second portion of the research involved adding an explicit treatment of warm-layer and cool-skin effects into a routine for estimating the bulk SST from satellite data. This part of research represented the primary contribution of Dr. Gary Wick. An accuracy comparison was performed between two different bulk SST algorithms. The traditional approach used only direct regression of the satellite brightness temperatures against in situ bulk SST measurements and, therefore, did not explicitly treat variability in the warm layer and cool skin. The second routine used models to determine the magnitude of the cool skin and any diurnal warming at each satellite pixel. The second approach offered the advantage of more directly treating the physics of the measurement problem but also incorporated the disadvantages of requiring more input data and introducing additional model uncertainties into the retrieval. The comparison was performed using GOES data because of its ability to monitor surface temperature throughout the diurnal cycle. The greatest accuracy improvement from using the second method was expected during the day when diurnal warming and the winds can lead to large variability in the near-surface temperature profile.

The novel approach of the second retrieval method warrants further description. The basic steps are as follows: 1) At each match location to be used in the derivation of the algorithm, a skin temperature is computed from a measured bulk SST and the modeled temperature difference between the bulk and skin temperatures. 2) The satellite brightness temperatures are regressed against these skin temperature estimates to derive a satellite skin SST algorithm. 3) The satellite skin SST algorithm is used to compute skin temperature measurements throughout the coverage region from the measured brightness temperatures. 4) At each pixel, bulk SST estimates are then computed from the satellite skin temperature measurements and modeled bulk-skin temperature differences. 5) At independent validation locations, these bulk SST estimates are compared with actual bulk SST measurements and the accuracy of the procedure is determined.

The model used to relate the bulk and skin temperatures incorporates components for both the warm layer and cool skin. The temperature change across the cool skin is computed using the parameterization of Wick et al. (1996). The temperature profile from the base of the skin layer to the depth of the bulk SST is predicted using a modified version of the one-dimensional, second-moment turbulence closure mixed layer model of Kantha and Clayson (1994). To compute the temperature differences, the wind speed and net and solar heat flux are required as additional inputs. The wind speed and heat flux components were taken from the NCEP/NCAR 40-year reanalysis project (Kalnay et al., 1996). Uncertainties in both the numerical models and the wind speed and heat flux fields contribute to errors in the final bulk SST estimates.

The results of the comparison showed that the accuracy improvements associated with the better physical treatment of the near-surface layer were largely balanced by uncertainties in the models and the extra required input fields. The overall accuracy of the two approaches was essentially the same. While no significant accuracy improvement was observed in this experiment, the results are still encouraging because earlier efforts had actually shown a decrease in accuracy when estimates of temperature differences across the skin layer were included. With further improvements to the models and input fields in the future, significant improvements in the accuracy of satellite bulk SST estimates are expected.

These results were incorporated in a manuscript submitted to the Journal of Atmospheric and Oceanic Technology in December, 2000 (Wick et al., 2001). Final revisions have now been completed and a decision on the status of the paper is expected soon. A complete copy of this manuscript is included at the end of this report. All work on this portion of the project was completed by the end of the initial grant and no extension funds were used.

Conclusions

Through this project, several important steps were taken to help determine whether the accuracy of satellite measurements of SST could be improved by explicitly accounting for the complex temperature gradients at the surface of the ocean associated with the cool skin and diurnal warm layers. To conclude, we include a list of the most significant accomplishments of this research:

- Two different low-cost radiometers were designed and developed for the purpose of collecting large numbers of in situ observations of the radiometric skin temperature of the ocean from ships of opportunity.
- The first of these radiometers was successfully deployed on two different research cruises.
- These data were used in the Ph.D. dissertation of Dr. Sandra Castro to significantly refine models for the temperature difference across the cool skin. These results are currently being included in a manuscript for journal publication.
- Experience gained from the development and deployment of the first radiometer was applied to the development of a second, more robust design. In addition to the development of the second radiometer funded by this project, Dr. Donlon also applied the experience to another radiometer he developed independently after leaving the University of Colorado.
- Initial laboratory testing on the second radiometer has been completed and preparations are being made for an extended rooftop test.
- A new satellite bulk SST retrieval method that explicitly accounts for the oceanic skin layer and near surface warming was developed and compared against a traditional

bulk SST algorithm derived directly from regression against in situ bulk SST measurements.

- The results of this comparison are included in a manuscript to appear in the Journal of Atmospheric and Oceanic Technology. The complete manuscript is included as an attachment to this report.

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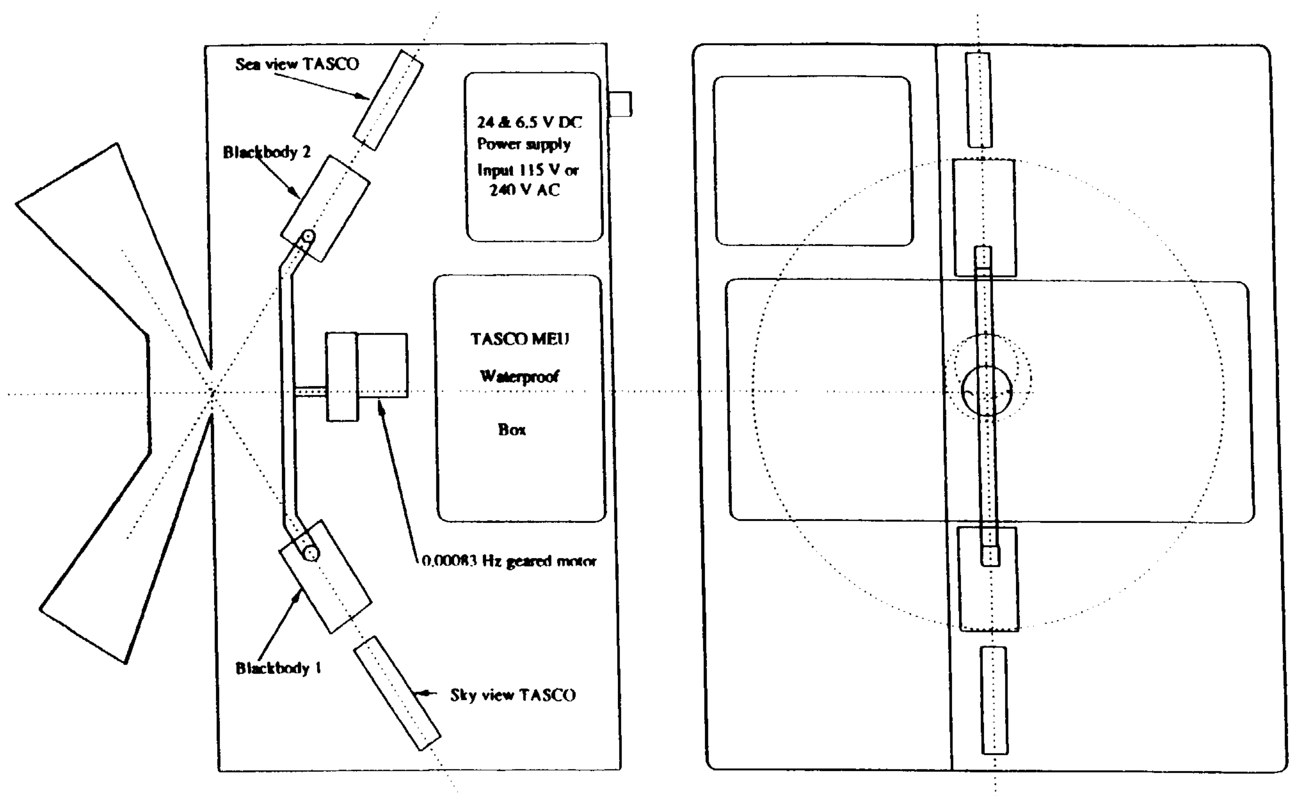
Figures

Figure 1. Schematic illustration of the SOSSTR measurement package.

Figure 2. Sample of the raw measurements from the sea and sky-looking radiometers in the SOSSTR during one day of the 1998 cruise on the RRS James Clark Ross. The measurements illustrate the calibration cycles with the warm and ambient blackbodies that must be used in the data processing.

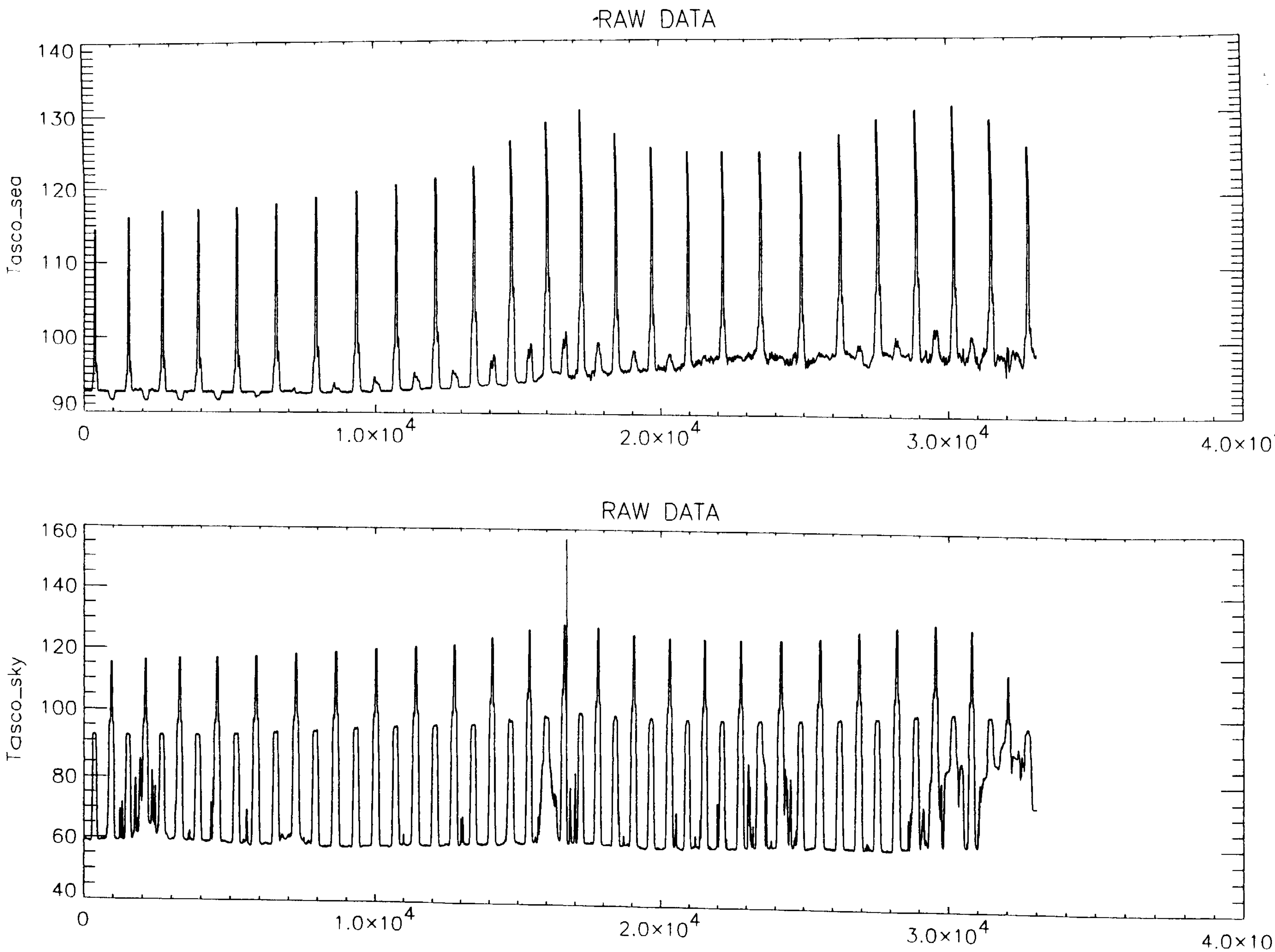
Figure 3. Final time series of calibrated and sky reflection corrected skin SST measurements along with the corresponding wind speed and net air-sea heat flux from the RRS James Clark Ross cruise. Data are only shown where all measurement were available and reliable.

Figure 4. Comparison of bulk-skin temperature difference estimates predicted using the new model of Castro (2001) with the corresponding measurements obtained using the SOSSTR. The results illustrate the scientific usefulness of the data and the consistency of the results with other radiometers.



Ship of oppotunity sea surface temperature radiometer (SOSSTR)
C. J. Donlon March 1997

Figure 1



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RAW DATA
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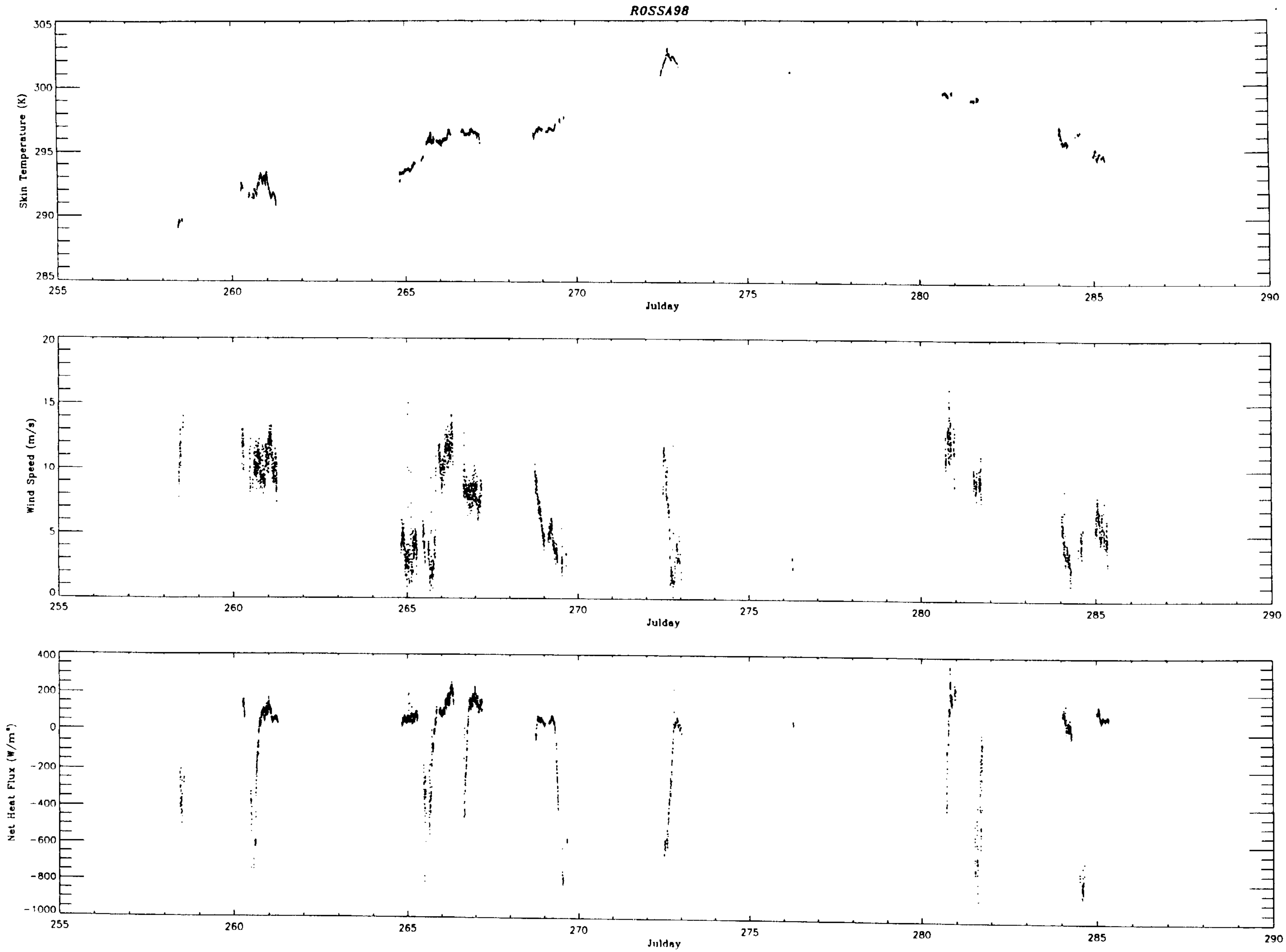
Figure 2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Julday
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5
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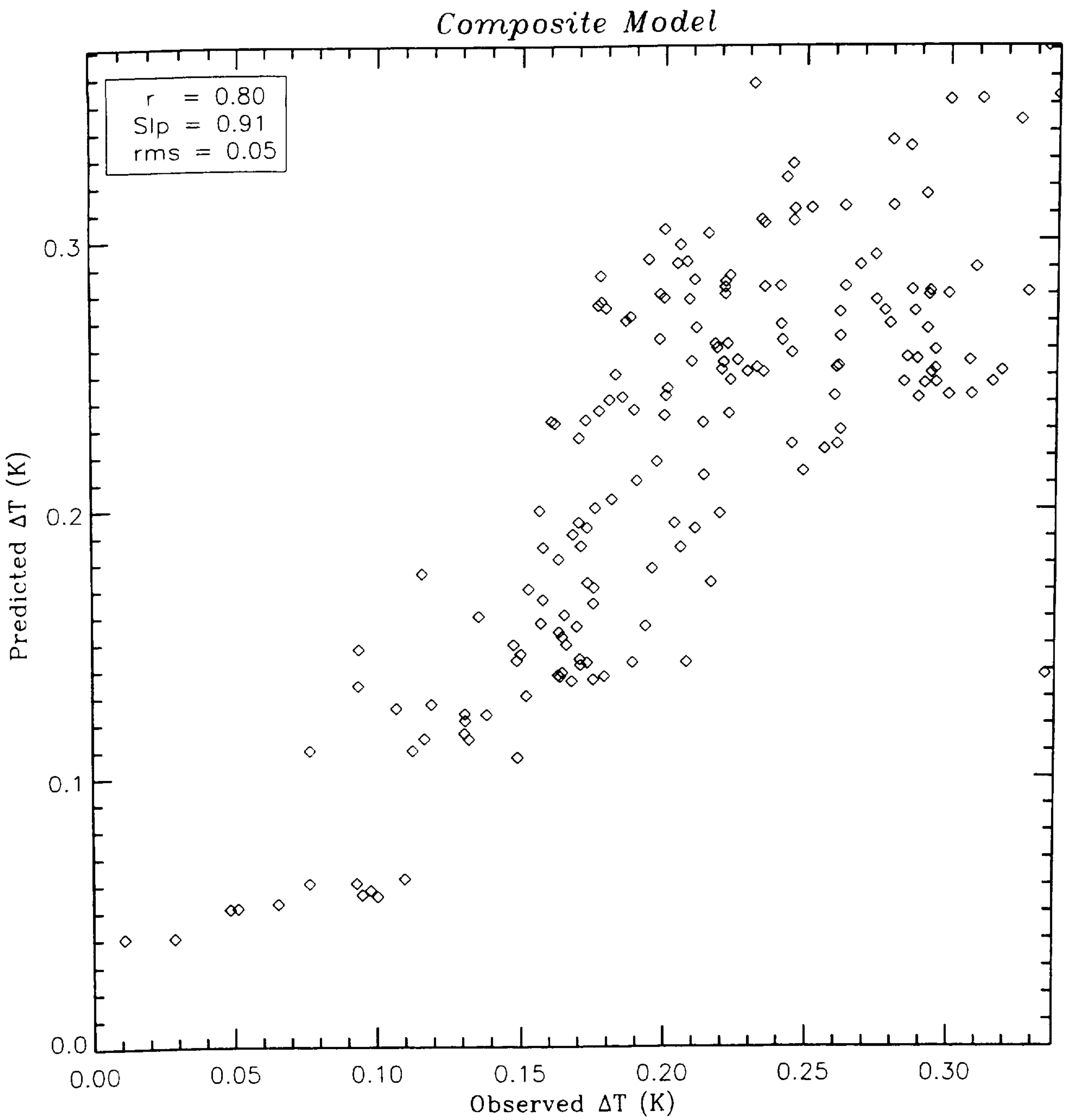
Figure 3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Slp = 0.91
rms = 0.05
Predicted ΔT (K)
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0.2
0.3
0.00
0.05
0.10
0.15
0.20
0.25
0.30
Observed ΔT (K)

Figure 4