Improving Satellite Retrieved Infrared Sea Surface Temperatures in Aerosol Contaminated Regions

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IMPROVING SATELLITE RETRIEVED INFRARED SEA SURFACE TEMPERATURES IN AEROSOL CONTAMINATED REGIONS

By

Bingkun Luo

A THESIS

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IMPROVING SATELLITE RETRIEVED INFRARED SEA SURFACE
TEMPERATURES IN AEROSOL CONTAMINATED REGIONS

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Infrared satellite observations of sea surface temperature (SST) have become essential for many applications in meteorology, climatology, and oceanography. Infrared satellite instruments passively measure the infrared energy reflected and emitted by the Earth's surface, which is then modified by the intervening atmosphere. Tropospheric aerosol concentrations increase infrared signal attenuation and affect the accuracy of infrared satellite SST retrievals. Satellite-derived skin SST with measurements from the Marine-Atmospheric Emitted Radiance Interferometer (M-AERI) deployed on ships during the Aerosols and Ocean Science Expeditions (AEROSE) and quality-controlled, collocated subsurface drifter temperatures. Satellite skin SSTs with any possible cloud contamination were removed from the dataset then the remaining measurements were temporally and spatially collocated with the in-situ SST (skin and bulk) measurements. With in-situ SST_{skin} and filtering of cloud contaminated data, results indicate that, in this region, SST_{skin} retrieved from MODIS (Moderate Resolution Imaging Spectroradiometer) aboard the Aqua satellites have cool biases compared to shipboard radiometric measurements. There is also a pronounced negative bias in the Saharan outflow area that can introduce SST_{skin} errors >1 K at aerosol optical depths > 0.5. In this study, a new method to derive night-time Dust-introduced SST Difference Index (DSDI) algorithms
based on simulated brightness temperatures at infrared wavelengths of 3.9, 8.7, 10.8 and 12.0 μm, is derived using Radiative Transfer for TOVS (RTTOV). Algorithm for MODIS measurements were derived by regression of the difference between the MODIS SST_{skin} and the in-situ measurements against the DSDI. The biases and STD are reduced by 0.25K and 0.19K after the DSDI correction. The goal of this study is to understand better the characteristics of aerosol effects on satellite retrieved infrared SST, and to derive empirical formulae for improved accuracies in aerosol-contaminated regions.

This organized as follows. After an introductory section, part 2 describes the background of SST_{skin} retrievals and accuracy, and includes a review of published papers on aerosol corrections. Because this research will use an Radiative Transfer model, it will also introduce the Radiative Transfer Equation in this section. The experiment location, duration, instruments used for data collection are discussed in section 3. Our technical approach is given in section 4. The results derived from numerical simulations and applications to MODIS Match-up database are summarized in section 5. Section 6 summarizes the work and discusses work in the future.
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Table of Contents

Chapter 1 Introduction and Motivation ................................................................. 1
Chapter 2 Background ......................................................................................... 4
  2.1 Sea surface temperature definition ............................................................. 4
  2.2 SST_{skin} retrievals and accuracy ............................................................... 7
  2.3 Previous aerosol corrections to SST_{skin} .................................................. 9
  2.4 The radiative transfer equation ................................................................. 11
Chapter 3 Data and Analysis Fields ................................................................. 16
  3.1 Analysis fields .......................................................................................... 16
  3.2 In-situ datasets (M-AERI) ........................................................................ 16
  3.3 In-situ datasets (drifters and buoys) ........................................................... 19
  3.4 Satellite datasets (MODIS, SEVIRI, CALIPSO) ....................................... 20
  3.5 Model datasets (MERRA-2) ..................................................................... 22
Chapter 4 Technical Approach and Methodology ............................................. 26
  4.1 Dust spectral optical properties ................................................................. 28
  4.2 RTTOV simulations ................................................................................. 32
  4.3 Match-up summary ................................................................................. 37
  4.4 SEVIRI error distribution ........................................................................ 39
  4.5 MODIS differences with AOD ................................................................. 41
  4.6 SEVIRI differences with AOD ................................................................. 45
Chapter 5 Results ............................................................................................... 48
  5.1 RTTOV model simulation of aerosol dust ................................................. 48
  5.2 RTTOV model simulation of satellite zenith angle ..................................... 53
  5.3 Derivation of a MODIS correction algorithm using MUDB ....................... 55
  5.4 Validation of this approach ..................................................................... 63
Chapter 6 Summary and Future Work ............................................................. 66
References .......................................................................................................... 69
List of Figures

Figure 1. Distribution of Terra MODIS SST matchups with in-situ drifting buoy measurements (Minnett et al. 2016). The color means the SST difference between MODIS SSTs with in-situ measurements from drifting buoy. ................................. 2

Figure 2. Idealized temperature profiles of the near surface layer (~10m) of the ocean during (left) night time as well as daytime during strong wind-driven vertical mixing conditions and (right) daytime during low wind and sunny conditions................. 5

Figure 3. Radiative effects due to the absorption and re-emission of infrared photons ........ 9

Figure 4. Relationship between particle size, radiation wavelength and scattering behavior for atmospheric particles. Dashed lines represent rough boundaries between scattering regimes. (Petty, 2004) ................................................................ 14

Figure 5. Left: The M-AERI is mounted on port side railing of the ship. Right: Unenhanced photograph of the forward level-2 of the NOAA ship Ronald H. Brown, taken during AEROSE-III, on the afternoon of 13 May 2007, during the major Saharan dust outflow pulse. (Nalli et al. 2011)......................................................... 17

Figure 6. Cruise tracks of the NOAA Ship Ronald H. Brown in the tropical North Atlantic Ocean during AEROSE cruises. The color indicates the SST_{skin} ...................... 18

Figure 7 Drifter before deployment. Source: http://www.aoml.noaa.gov/phod/dac/gdp_drifter.php .............................................. 19

Figure 8. Location of drifter on Oct 16, 2017. Different colors mean different deploying country. Source: http://www.aoml.noaa.gov/phod/dac/index.php................................................ 20

Figure 9. CALIPSO attenuated backscatter data over Saharan Outflow areas Time:2017-01-08 15:25:58. From NASA Langley ASDC CALIPSO Browse Images Systems at https://www-calipso.larc.nasa.gov/products/lidar/browse_images/production/ ....... 22

Figure 10. MERRA-2 input SST data during a dust break on Aug.18 2017. .................... 25

Figure 11. MERRA-2 input AOD data during a dust break on Aug.18 2017. .................... 25

Figure 12. Analysis flow diagram..................................................................................... 27

Figure 13. Real and imaginary parts of the refractive indices of different particle optical properties are given for each wavelength. (Hess et al. 1998). Four gray stripes in the background means MODIS AQUA infrared channels 20 (λ=3.8 μm), 29 (λ=8.9 μm), 31 (λ=11 μm), 32 (λ=12 μm). ................................................................................... 29

Figure 14. Real part LW refractive index of dust by Di Biagio et al. 2017, the magnitude is observed to vary region to region, and the water refractive index is different from aerosol dust near some spectral range.............................................................. 30

Figure 15. Imaginary part of LW refractive index of dust by Di Biagio et al. 2017. The magnitude of dust refractive index is observed to vary region to region, and the water refractive index is different from aerosol dust near some spectral range. ..... 30

Figure 16. The radiative impact of the Continental Clean aerosol type (black curve) and the error introduced by the scaling approximation (red curve) for the tropical profile for two different aerosol number densities (Matricardi, 2015).......................... 33

Figure 17. MERRA-2 input values of RTTOV ................................................................. 36

Figure 18. MODIS Aqua SST Difference near Saharan Outflow area, the quality flag values of MODIS Aqua are 0, 1, 2............................................................................. 39

Figure 19. SEVIRI and MAERI data; the x-axis is the time values of the SEVIRI MUDB. The SEVIRI and MAERI agree well and the SST difference is between ±2K. The
histogram is the SST difference that grouped into bins of every 1K difference, the MAERI derived SST is cooler than M-AERI SST as shown in the histogram. 

Figure 20. SEVIRI SST difference distribution with the track of ship. The color means the difference between SEVIRI SST and M-AERI SST skin. The red boxes are Saharan Dust outbreak area, there are significant negative SST difference between them in this area.

Figure 21. SST differences (MODIS SST skin between in-situ buoys SST) with MODIS Aerosol Optical Depth. This scatter plot is colored by the density of points. The red line is the fitted line of these points.

Figure 22. Column Integrated Attenuated Backscatter with Aerosol Optical Depth, the fitted red line clearly shows the aerosol in the atmosphere will attenuate backscatter signal.

Figure 23. MODIS SST skin Difference with Layer Altitudes (Left: Top Altitude. Right: Base Altitude).

Figure 24. SST Difference with Number of Aerosol Layers. The SST difference increases with number of aerosol layers. The fitted red line shows the SST difference will be more negative with increasing of number of aerosol layers.

Figure 25. SEVIRI differences with respect to M-AERI with AOD, the SST difference increases with AOD.

Figure 26. SEVIRI differences with AOD. The left Y-axis means the MODIS SST minus in-situ measurement SST, the right Y-axis means the MODIS derived AOD. As shown in the green ovals, when there is large AOD, the strong aerosol in the atmosphere causes more negative SST difference.

Figure 27. SEVIRI SST differences respected with ECMWF with AOD. Left is the SST difference between ECMWF model data and SEVIRI SST data, there is negative bias near Sahara outflow area as shown in right figure where the AOD is relatively high. The MODIS AOD daily sampling data offered here have large data gaps due to presence of clouds and the path of the Aqua satellite.

Figure 28. Changes in BT difference versus AOD assuming a layer of aerosol evenly distributed between 2 and 3 km altitude. (a) and (b) use Haywood optical properties. (c) and (d) use OPAC dust parameters. (Merchant et al. 2006)

Figure 29. Changes in BT difference versus Aerosol Concentrations. With the increasing of the aerosol concentrations, the BT difference between different channels will decrease of increase. This characteristic can be used to deduce the DSDI formula.

Figure 30. BT difference with SST skin difference, the color indicate different values of aerosol related SST skin differences.

Figure 31. Derived DSDI and its relationship with SST skin difference and aerosol concentration. The left figure clearly shows the aerosol layer causes negative SST difference and the right figure shows how DSDI is related to the aerosol layer and can be used to correct the SST skin difference.

Figure 32. Difference in simulated SST skin when aerosols are present or not. The SST skin difference is related to the aerosol distribution.

Figure 33. Derived Dust-introduced SST Difference Index. Compared to Figure 29, the derived DSDI distribution is clearly related to the SST skin difference.
Figure 34. Satellite Zenith Angle is the angle between the straight line from the viewing point to the satellite and the line perpendicular to the viewing point. From: https://definedterm.com/satellite_zenith_angle ........................................................ 53

Figure 35. SST Difference with satellite view angle (Ignatov et al. 2016). The data that are used are from NOAA16, NOAA17, NOAA18, NOAA19 and METOPA satellite, the y-axis is the SST difference between satellite and buoys. ........................................ 54

Figure 36. RTTOV simulated SST skin difference as a function of Satellite Zenith Angle. Based on simulated 300 data points of nighttime BT at 36 view angles (0° to 72°) under aerosol-free conditions. ................................................................................... 54

Figure 37. Left: scatter plot of the SST skin difference with BT3.8-BT12 and BT11-BT12, color means the SST skin difference, it can be used to represent the aerosol introduced SST skin difference. Right: Derived DSDI with BT difference, corresponding to the left picture and it can be used to correct the SST skin difference. ......................... 55

Figure 38. BT Difference with SST skin difference, this scatter plot takes the satellite view angle term S0 into account. Color indicates SST skin difference. It can easily distinguish the SST skin difference using the BT difference after adding satellite view angle term .................................................................................................................. 56

Figure 39. Distribution of empirically derived DSDI. The DSDI value is relatively high in the Saharan dust outbreak area. In other words, the DSDI can be used to represent the SST difference with respect to drifter measurements and can be used to correct the MODIS SST skin retrieval algorithms.......................................................... 57

Figure 40. Empirical derived DSDI with SST skin Difference. ........................................ 58

Figure 41. Empirically derived DSDI>0.8 with SST skin difference. The fitted line clearly shows when DSDI>0.8, the relationship between DSDI and SST difference can be used to correct the aerosol introduced bias. .............................................................. 59

Figure 42. Difference between Aqua MODIS SST with in-situ buoy SST before DSDI correction. ................................................................................................................. 60

Figure 43. Difference between Aqua MODIS SST with in-situ buoy SST after correction. ................................................................................................................................... 60

Figure 44. The difference in SST skin between before and after aerosol correction. This aerosol correction term is high at Saharan dust outflow area. ........................................ 60

Figure 45. Histograms of the SST skin difference, before and after correction. The mean SST difference has decreased by an amount of 0.18K. There are a few points below -2K after correction. .............................................................. 61

Figure 46. Before and after correction the SST difference. Because this area is near the Saharan dust outflow area and the satellite retrieved SST is more likely to be affected by the dust aerosol in this region. ......................................................... 62

Figure 47. Histograms of the SST difference, before and after correction. Compared to Figure 42, there is a greater decrease of the SST difference by 0.26K. ...................... 63

Figure 48. Dust-introduced SST Difference Index applied to 20% of the data that were withheld in the derivation of the DSDI form and of the coefficients. ..................... 64

Figure 49. Difference between Aqua MODIS SST with in-situ buoy SST before correction (Withheld 20% of the data)........................................................... 65

Figure 50. Difference between Aqua MODIS SST skin with in-situ buoy SST after correction (Withheld 20% of the data). ............................................................ 65
Figure 51. RTTOV simulated effects show the altitude of the aerosol layer has an impact on the SST\textsubscript{Skin} retrieval. Different colors indicate different altitudes of the dust layers. With the increasing of aerosol height, the SST difference is more negative. 67
List of Tables

Table 1. Vertical temperature profile definition through the ocean surface layer .......... 6
Table 2. Satellite datasets .................................................................................................. 21
Table 3. MERRA-2 data used in this study ................................................................. 25
Table 4. Mineral transported aerosol type and layer depth ............................................ 34
Table 5. Statistics of errors of MODIS Aqua SST vs in-situ measurements. The mean SST bias increases with AOD. Especially when AOD>0.5, the mean SST bias can be larger than 1K as marked as red color in this table ............................................. 41
Table 6. Statistics of errors of Meteosat SEVIRI SST vs AOD ................................. 46
Table 7 Error analysis associated with developed DSDI ............................................ 57
Table 8. Error statistics according to MODIS quality flag .......................................... 61
Table 9. Statistics of the difference between MODIS Aqua SST and in-situ temperature in this region (between 90° W to 90° E and 20° S to 35° N.) ............................... 63
**Chapter 1 Introduction and Motivation**

Sea surface temperature (SST) derived from satellites is one of the key parameters in the research and prediction of climate variability and change, and for many other research and operational applications. Generating SST Climate Data Records, require an absolute temperature error of 0.1K and stability of better than 0.04K per decade (Ohring et al., 2005). Therefore, it is essential to quantify the errors and uncertainties of SST and obtain highly accurate satellite derived SST\textsubscript{skin}, and improve the accuracy in situations where there is evidence of systematic shortcomings in the retrieval algorithms.

NASA’s earth observation satellites enable a comprehensive set of measurements to improve our understanding of the earth system. The MODerate-resolution Imaging Spectroradiometer (MODIS) is a satellite-based visible/infrared spectroradiometer aboard the Earth Observing System Satellites Terra and Aqua to sense radiation of terrestrial, atmospheric, and oceanic phenomena. Terra and Aqua are polar-orbiting satellites and MODIS acquires data in 36 spectral bands, which provide important information for many research applications, including oceans (Esaias et al., 1998; Kilpatrick et al., 2015), and atmospheres (Remer et al., 2005; King et al., 2003). While our study, detailed below, was based on measurements of MODIS on Aqua, the improved SST\textsubscript{skin} retrieval accuracy will be applicable to measurements of other infrared radiometers on other satellites such as the Spinning Enhanced Visible and InfraRed Imager (SEVIRI) on the Meteosat Second Generation (MSG-3) satellites or the Visible Infrared Imaging Radiometer Suite (VIIRS) on NOAA-20.
Analysis of comparisons of MODIS SSTs with in-situ measurements from drifting buoys over the missions of Terra and Aqua show that, generally, mean biases are \( \sim 0.17 \, \text{K} \) and standard deviation \( \sim 0.25 \, \text{K} \). (Minnett et al. 2016). These are indications of the performance of the cloud screening and atmospheric correction algorithms. From the spatial distribution of the difference between MODIS derived SSTs and in-situ buoys temperatures (Figure 1), there is a pronounced negative difference in the Saharan outflow area. Szczodrak, et al. (2014) discussed the effects of anomalously low moisture layers on the accuracy of MODIS SST_{skin} and quantified these effects using data from measurements used during research cruises and numerical models. They found that for deep dry layers, the errors can be \( >1 \, \text{K} \). The retrieval errors depend on the characteristics of dry layers in the atmosphere. The altitude of the dry layers affects the sign of errors in the SST_{skin} retrieval. In the area of the Saharan Outflow, the dry layers are often
accompanied by dust aerosols. The absorption and re-emission of aerosol layers cause brightness temperatures derived from satellite infrared radiometers generally to be too cold, so an atmospheric correction algorithm is needed to reduce this cool bias (Závody et al., 1995).

Correcting aerosol related errors can also improve satellite coverage rather than just discarding the aerosol contaminated retrievals. Not only is this important for generating Climate Data Records, but for many other oceanographic and climate research topics. For example, the tropical Atlantic Ocean SST\(_{\text{skin}}\) distributions are indicative of changes in the ocean circulation, including the Atlantic Meridional Overturning Circulation (Liu and Minnett, 2015). SSTs and MODIS AODs, supported by upper ocean modeling, showed reductions in the SST\(_{\text{skin}}\) of up to 0.2 - 0.4 K simultaneously with, or shortly after, strong dust outbreaks (Martínez Avellaneda et al., 2010). The effects are not limited to a local ocean response, but extend through modifications to the upper-ocean heat content and the large-scale circulation to the entire Atlantic Ocean (Serra et al., 2014).

This research addresses the following questions:

- How are the errors in SST\(_{\text{skin}}\) dependent on the aerosol properties?
- How to improve the atmospheric correction algorithms in aerosol contaminated regions to reduce significantly the SST\(_{\text{skin}}\) errors?
Chapter 2 Background

2.1 Sea surface temperature definition

The term sea surface temperature is difficult to define precisely. The upper ocean temperature variability varies diurnally due to ocean turbulence, air-sea interaction and heating caused by the absorption of solar radiation. The Group of High Resolution SST Pilot Project (GHRSSST-PP) workshops provided a set of definitions that can be used to classify SST measured by various instruments. The temperature of the depth where there is no any diurnal signal is defined as the Foundation SST, the SSTskin changes corresponds to the surface temperature and this Foundation SST (Donlon et al. 2007).

The daily progression of the surface and subsurface warming and its dependence on environmental forcing, including wind and insolation, has been well documented (Gentemann et al. 2003, Stuart-Menteth et al. 2005). Much current SST related research uses in-situ measurements, these may vary by a few degrees depending on the depth of the thermometer and the effects of diurnal heating. After comparison of different measured temperatures, there are notable difference between infrared satellite derived temperature and the temperature measured by in situ instruments. So it is very important to know how the near-surface thermal structure of the ocean behaves in nature, and to understand the measuring depth and recognize the depth genre, whether it is ‘skin’, ‘subskin’ or ‘SST depth temperature’ (Donlon et al. 2002, Donlon et al. 2007, See Figure 2). In this study, the ship-based and satellite infrared radiometers will be used, these instruments represent the actual temperature of the water across a very small depth, approximately 20 micrometers, it is 'skin' temperature. This research will also use the
drifting buoy temperature data, it is typically called as SST or "bulk" SST, which means an in-situ measurement near the surface of the ocean.

Figure 2. Idealized temperature profiles of the near surface layer (~10m) of the ocean during (left) night time as well as daytime during strong wind-driven vertical mixing conditions and (right) daytime during low wind and sunny conditions.

Taken from: http://ghrsst-pp.metoffice.com/pages/sst Definitions/
### Table 1. Vertical temperature profile definition through the ocean surface layer

<table>
<thead>
<tr>
<th>Temperature Type</th>
<th>Depth</th>
<th>Measurement</th>
</tr>
</thead>
<tbody>
<tr>
<td>The interface SST (SS_int)</td>
<td>A theoretical temperature at the precise air-sea interface. The topmost layer of the ocean water and could be thought of as an even mix of water and air molecules.</td>
<td>Cannot be measured using current technology.</td>
</tr>
<tr>
<td>The skin SST (SST_skin)</td>
<td>The radiometric temperature measured by an infrared radiometer operating in the 10-12 micrometer spectral waveband. It represents the actual temperature of the water across very small depth of approximately 20 micrometers.</td>
<td>SST_skin measurements are subject to large potential diurnal cycle. Such as Infrared radiometers, MODIS or SEVIRI.</td>
</tr>
<tr>
<td>The sub-skin SST (SST_subskin)</td>
<td>The temperature at the base of the thermal skin layer. SST_subskin is the temperature of a layer ~1mm thick at the ocean surface.</td>
<td>SST_subskin can be measured by a microwave radiometer operating in the 6-11 GHz frequency range</td>
</tr>
<tr>
<td>SST_depth or SST(z)</td>
<td>It represents an in-situ measurement near the surface of the ocean that is typically reported simply as SST or &quot;bulk&quot; SST. These temperature observations are distinct from those obtained using remote sensing techniques and measurements at a given depth arguably should be referred to as 'sea temperature' (ST) qualified by a depth in meters</td>
<td>SST_depth can be measured by drifting buoy, moored buoy, thermosalinograph (TSG) systems aboard ships, Conductivity Temperature and Depth (CTD) systems, and various expendable bathythermograph systems.</td>
</tr>
<tr>
<td>The Foundation SST (SST_fnd)</td>
<td>The temperature of the water column free of diurnal temperature variability or equal to the SST_subskin in the absence of any diurnal signal.</td>
<td>SST_fnd cannot be directly measured using either microwave or infrared satellite instruments. It can be measured by in-situ Buoy, Ships</td>
</tr>
</tbody>
</table>

Taken from: http://ghrsst-pp.metoffice.com/pages/sst_definitions/

(Definitions of SST within the GHRSSST-PP, 2005).
2.2 SST$_{skin}$ retrievals and accuracy

IR observations are considered a skin SST measurement because the SST$_{skin}$ retrieval algorithms usually remove cloudy and aerosol-contaminated data, and SST$_{skin}$ in the infrared can be derived only in cloud-free conditions. The SST$_{skin}$ retrievals from infrared sensors have several sources of error and uncertainty, such as satellite zenith angle, cloud removal techniques, incorrect atmospheric transmission correction etc. The MODIS includes three mid-infrared (IR) channels with wavelengths close to 3.7\,\mu m, plus two at wavelength centered at 10.8\,\mu m and 12.0\,\mu m that can be used to derive SST$_{skin}$.

High tropospheric aerosol concentrations significantly modify infrared atmospheric radiative transfer, thus preventing the retrieval of accurate satellite SSTs using atmospheric correction algorithms designed to correct the effects of water vapor (May et al. 1992). It is sometimes difficult to distinguish between clouds and aerosols, and between clear sky and conditions with aerosols.

The new Version 6 AQUA and TERRA MODIS SST$_{skin}$ processing algorithm involves three extra correction terms, two additional satellite zenith angle corrections and a single term relating to a mirror side.

The updated forms of the algorithms are defined by Kilpatrick et al. (2014) to derive skin SST:

\[
SST_{sat} = a_0 + a_1 BT_{31} + a_2 (BT_{31}-BT_{32}) * T_{sfc} + a_3 (\sec (\theta)-1) * (BT_{31}-BT_{32})) + a_4 (\text{mirror. side}) + a_5 (\theta) + a_6 (\theta)^2
\]

Equation 1
\[ \text{SST}_{\text{sat}} = a_0 + a_1 \text{BT}_{22} + a_2 (\text{BT}_{22} - \text{BT}_{23}) + a_3 (\sec \theta - 1) + a_4 \text{mirror. side} + a_5 \theta + a_6 \theta^2 \]

*Equation 2*

The unit of the brightness temperatures is Kelvin. \(a_0\) etc are coefficients and that \(\text{BT}_{31}\) is the brightness temperature of channel 31 and \(\text{BT}_{32}\) is the brightness temperature of channel 32. In the current version 6, coefficients are estimated as a function of both month and latitude band. The goal of monthly coefficients is to reduce the residual seasonal effects in each hemisphere.

Empirical coefficients derived from buoy matchups may not reflect the conditions at locations where buoys data are sparse particularly in Polar Regions where the emissivity of the cold surface and a dry atmosphere can lead to an ineffective atmosphere correction algorithm. The coefficient estimations were made using a generalized linear model, run multiple times to create 72 sets of coefficients corresponding to 12 months times six latitude bands.

The operational SST_{skin} algorithm used in day and night conditions for MSG/SEVIRI (at present METEOSAT10) is also the (non-linear) NL algorithm (Walton et al. 1998) described by Geostationary Sea Surface Temperature Product User Manual version 1.5 (2016).
2.3 Previous aerosol corrections to $SST_{\text{skin}}$

*Figure 3. Radiative effects due to the absorption and re-emission of infrared photons*

The radiative effects due to the absorption and re-emission of infrared photons by aerosols in the atmosphere (Figure 3) will introduce the errors into infrared derived SST (Kidder and Vonder Haar, 1995). To better understand the effects of aerosol layer on satellite derived $SST_{\text{skin}}$, comparisons between data from various satellites and in-situ measurements have been carried out for many years. The dual-view approach of the Along Track Scanning Radiometer-2 (ATSR-2) reduced the sensitivity to aerosols along with the application of a simple statistical regression model of aerosol. Vázquez-Cuervo, et al. (2004) compared the ATSR-2 $SST_{\text{skin}}$ with AVHRR and plotted the difference maps. SST differences varied regionally and the largest was near west Africa. Arbelo et al. (2005) investigated Advanced Very High-Resolution Radiometer (AVHRR) derived SST errors using the Sea-viewing Wide Field-of-view Sensor (SeaWiFS) Aerosol Optical Thickness product. Pathfinder residual SST errors increased with SeaWiFS derived
aerosol optical thickness (AOT), the brightness temperature at bands 4 and 5 (10.30-11.30 µm and 11.50-12.50 µm) is related to AOT. The relationship between SST\textsubscript{skin} retrieval errors and regional aerosol patterns reflects inadequacies in the cloud screening or clear-sky atmospheric correction algorithm. The consequences of dust aerosols over the ocean is not limited to causing bias errors in infrared (IR) derived SST\textsubscript{skin} but also have geophysical consequences. Using surface measurements taken in the Cape Verde Islands, Gehlot et al. (2015) showed that the presence of Saharan Dust aerosols can result in a reduction of up to 200 Wm\textsuperscript{-2} in the surface insolation, the partially compensating effects of increased IR radiation at the surface is an order of magnitude smaller (Vogelmann et al., 2003). Since SST\textsubscript{skin} derived from microwave radiometers is immune to aerosol effects, a comparison of TMI (TRMM Microwave Imager; Kummerow et al., 1998). Although SSTs derived using microwave radiometry are not affected by aerosols, the derived fields lack the spatial resolution provided by IR radiometers, retrievals are contaminated within ~75 km of land and by satellite to satellite as well as geostationary reflected radio, and by radio frequency interference (RFI). Although RFI is more problematic over land and around Europe and the USA (Vine et al., 2016), Ascension Island in the tropical South Atlantic is a source of RFI that extends into the southern part of the region impacted by aerosols (Gentemann, C. L., 2015).

Thus, there are pressing regions to improve the accuracies of SST\textsubscript{skin} derived from satellites in aerosol contaminated conditions. Our focus is on improving the SST\textsubscript{skin} retrievals from infrared radiometers.
2.4 The radiative transfer equation

Emission, absorption and scattering are three main physical interactions of the aerosol in the atmosphere. Aerosols in the atmosphere have three physical radiative influences on the signal measured on satellites: (1) The infrared emission of the aerosol particle at the same wavelength as the incident radiation will cause an increase of isotropic radiation from the aerosol layer. (2) The absorption of upwelling radiation by aerosol particles corresponds to an attenuation for upward-propagating radiation at the top of the atmosphere. (3) The scattering of the radiation by the aerosol particle in other directions than the original beam causes attenuation of the radiation at the top of atmosphere (Vidot, 2015).

The spectral radiance emitted by an object considered as a blackbody is determined by the Planck’s Law which depends on the temperature and on the wavelength, which is written as:

\[ B_{\text{flux}}(\lambda, T) = \frac{2\pihc^2}{\lambda^5} \frac{1}{e^{\frac{hc}{\lambda kT}} - 1} \]

*Equation 3*

where \( B_{\text{flux}} \) is the blackbody radiance, \( k \) is the Boltzmann constant, \( c \) is speed of light in a vacuum, \( h \) is the Planck constant, and \( T \) is the temperature. The unit of \( B_{\text{flux}}(\lambda, T) \) is \( \text{W} \cdot \text{sr}^{-1} \cdot \text{m}^{-3} \). This is Planck’s Law in the wavelength domain, which can be converted into frequency domain.

The blackbody will emit the radiance of:
\[ B(T) = \int_{\lambda_1}^{\lambda_2} B(\lambda, T) d\lambda \]

**Equation 4**

Because \( c = \nu \lambda \), so \( \frac{d\lambda}{d\nu} = \frac{c}{\nu^2} \), obtain

\[ \int_{\lambda_1}^{\lambda_2} B(\lambda, T) d\lambda = \int_{\nu_1}^{\nu_2} B(\nu, T) \frac{c}{\nu^2} d\nu \]

**Equation 5**

By substituting in equation 5 and rearranging. When calculated from the wavelength \([\lambda_1 \lambda_2]\) over the frequency \([\nu_1 \nu_2]\), then can obtain Planck distribution in frequency:

\[ B(\nu, T) = \frac{2h\nu^3}{c^2} \frac{1}{e^{\frac{h \nu}{kT}} - 1} \]

**Equation 6**

The thermal radiation energy emitted by the surface of a material is emissivity, and the radiation absorbed at the surface of a material is absorptivity. The emission emissivity of a surface equals absorptivity according to Kirchhoff’s Law. If consider an isolated system with two bodies in thermal equilibrium, one a blackbody and the other one is non-blackbody. The blackbody will emit a quantity \( B \) whereas the non-blackbody will emit a fraction \( \varepsilon \) of \( B \), the non-blackbody is the only source of reflection so that we can get

\[ B = \varepsilon B + r B \]

**Equation 7**

\( r \) is the fraction of reflectivity, \( \varepsilon \) is the fraction of emissivity, simplifying,
\[ 1 = \varepsilon + r \]

Equation 8

Because the total of reflectivity \( r \), absorptivity \( \alpha \), and transmittance \( \tau \) equal to 1, and the system is isolated, the transmittance is null, so \( r = 1 - \alpha \),

Then obtain

\[ 1 = \varepsilon + (1 - \alpha) \]

simplifying of Kirchhoff’s Law is

\[ \varepsilon = \alpha \]

Equation 9

The particle size also has an effect on the scattering component, the significance of this effect is given by the size parameter \( x \):

\[ x = \frac{2\pi r_{rad}}{\lambda} \]

Equation 10

where \( \lambda \) is the wavelength and \( r_{rad} \) is the particle radius. In the thermal IR region and Near IR region, scattering from dust aerosol is not negligible whereas in the MW region, scattering effects of aerosols are negligible. The particle radius, radiation wavelength and scattering behavior for atmospheric particles relation are shown in Figure 4.
Figure 4. Relationship between particle size, radiation wavelength and scattering behavior for atmospheric particles. Dashed lines represent rough boundaries between scattering regimes. (Petty, 2004)

The clear-sky infrared RTE is based on the Schwarzschild’s equation when considering a homogeneous plane-parallel non-scattering atmosphere. The Schwarzschild’s equation is given as:

\[ \mu \frac{dR(\mu)}{dz} = -k_a R(\mu) + k_a B(T) \]

Equation 11

Where \( k_a \) is the spectrally-dependent absorption coefficient of the atmospheric layer and \( B(T) \) is the Planck function of the atmospheric layer of temperature \( T \). \( R(\mu) \) is the radiance emitted by intensity \( \mu \). The solution of the Schwarzschild’s equation...
provides the clear-sky top-of-atmosphere (TOA) full infrared radiative transfer equation which represents the surface of earth and atmosphere’s radiance that will reach to the satellite:

$$R_{ctr}(\lambda, \theta) = \varepsilon(\lambda, \theta)B(T, \lambda)\tau_{sfc}(\lambda, \theta) + \int_{\tau_{sfc}}^{1} B(T, \lambda)\,d\tau + \left[1 - \varepsilon_{sfc}(\lambda, \theta)\right]\tau_{sfc}(\lambda, \theta)L_d$$

*Equation 12*

The first term on the right-hand side of Eq. 13, $\varepsilon(\lambda, \theta)B(T, \lambda)\tau_{sfc}(\lambda, \theta)$, is the total infrared radiation that reaches to the satellite, which will be a function of emissivity of target modified Planck’s distribution, where $\varepsilon(\lambda, \theta)$ is the emissivity related to viewing angle $\theta$ and wavelength $\lambda$, $B(T, \lambda)$ is the blackbody spectral radiance, and $\tau_{sfc}(\lambda, \theta)$ is the surface to space transmittance depended on viewing angle $\theta$ and wavelength $\lambda$.

The second term on the right-hand side of Eq. (13), $\int_{\tau_{sfc}}^{1} B(T, \lambda)\,d\tau$, is the upwelled radiance emitted by the atmosphere and it can be calculated by integrating emitted radiance from each atmospheric layer from the surface to the satellite.

The third term is the surface reflected radiance, because the atmospheric emitted downward radiance may be reflected toward the satellite, where $L_d$ is the downward surface irradiance emitted by the atmosphere.
Chapter 3 Data and Analysis Fields

This chapter describes the experiment location, duration, instruments used for data collection and techniques used for data analysis.

3.1 Analysis fields

The study methods include analysis of in-situ data, satellite data and modeled fields. Ship-based measurements were taken during cruise of AEROSE, a series of tropical Atlantic Ocean cruise campaigns. This research will use the in-situ datasets from 2006 to 2015. The satellite-derived SSTs are from MODIS on board Terra and Aqua and from SEVIRI on Meteosat between 2006 to 2016. The reanalysis model datasets from the NASA Modern-Era Retrospective analysis for Research and Applications, Version 2 (MERRA-2) will be used as data fields for the RTTOV model simulations during Aug 18, 2017 12:00 AM, as during this time there is a strong Sahara dust outbreak. Considering the Sahara dust area, the research area is between 90° W to 90° E and 20° S to 35° N.

3.2 In-situ datasets (M-AERI)

One of the difficulties in deriving an aerosol correction algorithm for \( \text{SST}_{\text{skin}} \) is the shortage of accurate in-situ data. To study the effects of aerosol layers on satellite derived \( \text{SST}_{\text{skin}} \), it is important to have high spatial and temporal resolution in-situ data which cover multiple locations and span considerable lengths of time, then these high accuracy in-situ data can be used to get the bias of the satellite data. These data should also be accompanied by ancillary environmental data measurements such as Light
Detection and Ranging (LIDAR) to provide aerosol layer data or radiosonde to provide dry layer data.

This study will utilize measurements of the Marine-Atmospheric Emitted Radiance Interferometer (M-AERI) (Figure 5), a dataset of multi-location in-situ skin sea surface temperature measurements that satisfy the above requirements. The M-AERI provides measurements of well-calibrated atmospheric and oceanic emission spectra (Minnett et al. 2001). From the M-AERI spectra, a number of critical geophysical state parameters can be derived, including high-accuracy radiometric sea surface skin temperature and IR spectral emissivity of the sea surface. The IR brightness temperature (centered at 3.7, 11, and 12 μm, respectively) measurements from the sea view are corrected for sky radiance reflected at the sea surface and direct and reflected atmospheric emission from the air between the M-AERI and the sea surface are representative of the ocean skin temperature, SSTskin. The M-AERI data are provided by RSMAS, University of Miami.

Figure 5. Left: The M-AERI is mounted on port side railing of the ship. Right: Unenhanced photograph of the forward level-2 of the NOAA ship Ronald H. Brown, taken during AEROSE-III, on the afternoon of 13 May 2007, during the major Saharan dust outflow pulse. (Nalli et al. 2011).
Because these in-situ cruise data are in a region with aerosols, it is feasible to use the in-situ data to improve our understanding of how aerosol layers affect $SST_{\text{skin}}$ retrievals. Figure 6 shows the M-AERI data from the AEROSE on board the NOAA Ship Ronald H. Brown. AEROSE is a multidisciplinary series of field campaigns designed to acquire simultaneously in situ and remotely sensed data during intensive observing.
periods (Nalli, et al. 2006), which can be used to characterize the radiation in IR impact of Saharan dust outflows over the Atlantic Ocean.

### 3.3 In-situ datasets (drifters and buoys)

NOAA established the in-situ sea surface temperature (SST) Quality Monitor (iQuam) to support the validation of satellite and blended SST products (Xu and Ignatov, 2016). Data from iQuam, which consists of quality-controlled measurements from drifters, moored buoys and ships, will be used here. The AOML drifter consists of a surface buoy and a subsurface drogue, attached by a long, thin tether as shown in Figure 7. The surface float diameters range around 35cm, and they contain batteries; a satellite data transmitter; a thermistor to measure sea surface temperature; and other instruments measuring barometric pressure, wind speed and direction etc. The drogue is centered at 15 meters beneath the surface to measure mixed layer currents in the upper ocean. The temperature sensor near the bottom of the buoy measures SST at a nominal depth of 20cm, but the exact depth depends on surface wave conditions and the entire float may be temporarily submerged. The distribution of the drifter is shown in Figure 8. Moored buoys are the weather sentinels of the sea and are deployed in the coastal and offshore waters. The Moored buoys data are from National Data Buoy Center by NOAA.

![Drifter before deployment](http://www.aoml.noaa.gov/phod/dac/gdp_drifter.php)
3.4 Satellite datasets (MODIS, SEVIRI, CALIPSO)

This study focuses on the satellite-derived SST$_{skin}$ from MODIS on board Aqua and SEVIRI on board Meteosat satellites from 2006 to 2016. Daily files were downloaded from the Long-Term Steward-ship and Reanalysis Facility (LTSRF) of the Group for High Resolution Sea Surface Temperature (GHRSSST) (Donlon et al. 2007). Daytime SST$_{skin}$ were from the MYD28L2/MOD28L2 datasets, MYD was MODIS on Aqua and MOD was MODIS on Terra. The thermal-infrared SST$_{skin}$ data were retrieved by nonlinear SST$_{skin}$ algorithms, NLSST (Walton et al. 1998, Brown et al. 1999; Kilpatrick et al. 2015). Aerosol optical depth (AOD) data were taken from MOD04L2 and MYD04L2 datasets, calculated by the ‘Deep Blue’ (DB) algorithm (Hsu et al., 2004).
The Level 1B products contain the calibrated data used by other software applications to construct the products or images. For MODIS radiances data, this research used MYD021KM Level 1B Calibrated Radiances to calculate brightness temperatures in the appropriate spectral bands. This dataset contains calibrated and geolocated at-aperture radiances for 36 discrete spectral bands located in the 0.4 µm to 14.4 µm region of the electromagnetic spectrum. The temporal resolution is twice per day and the spatial resolution is 1 km. These data are converted to geophysical units of W*(m² µm sr)⁻¹.

Data from the SEVIRI on the MSG-3 satellites were used for the Eastern Atlantic Region. Meteosat operates in geostationary orbit, 36000 km above the equator, continually viewing large areas of the Atlantic and provides data for climate monitoring and research at approximately 5 km resolution with a 15-minute repeat sampling. SEVIRI has 12 spectral channels to observe the Earth, eight of these channels are in the thermal infrared providing temperature information. SSTskin data are calculated at full resolution on a hourly basis.

Table 2. Satellite datasets

<table>
<thead>
<tr>
<th>Sensor and processing level</th>
<th>Temporal resolution</th>
<th>Spatial resolution</th>
<th>Area</th>
</tr>
</thead>
<tbody>
<tr>
<td>MODIS on Aqua Level 2</td>
<td>Twice a day. Satellite overpass time is at about 1:30 AM and 13:30 PM LST.</td>
<td>0.01°</td>
<td>Global</td>
</tr>
<tr>
<td>Meteosat-8/10 Level 3C</td>
<td>Every hour</td>
<td>0.05°</td>
<td>60°S - 60°N</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>60°W - 60°E</td>
</tr>
</tbody>
</table>
To study the vertical structure of aerosols, Cloud-Aerosol LIDAR and Infrared Pathfinder Satellite Observation (CALIPSO) datasets were used. LIDAR data from Cloud-Aerosol Lidar with Orthogonal Polarization (CALIOP) is particularly suitable for measuring the characteristics and physical mechanisms of aerosol layers. CALIPSO provides column aerosol optical depth, column integrated attenuated backscatter, layer base and top altitudes, number of layers etc. (Figure 9). The CALIPSO data are limited to measurements along the sub-satellite track as the LIDAR is directed at nadir.

3.5 Model datasets (MERRA-2)

Reanalysis data, which assimilate meteorological station, buoy, ship and satellite data, may provide an accurate representation of the SST in the Saharan Outflow area. What is more, the reanalysis ocean surface and atmospheric fields are internally consistent. The reanalysis model datasets from NASA Modern-Era Retrospective analysis
for Research and Applications, Version 2 (MERRA-2) will be used. These data are available through the Goddard Earth Sciences (GES) Data and Information Center (DISC) at http://disc.sci.gsfc.nasa.gov/mdisc/.

The MERRA-2 reanalysis model data were generated using the Goddard Earth Observing System (GEOS) data assimilation system (DAS) by NASA's Global Modeling and Assimilation Office (GMAO) Data Assimilation System Version 5.12.4., covering the earth observation data from 1980 to the present (Gelaro et al., 2017). The GEOS-5 model resolution of MERRA-2 is approximately 0.625° in longitude and 0.5° in latitude and MERRA-2 has a one-hourly or three-hourly output frequency. The model data have 72 hybrid sigma-pressure layers. This sigma coordinate system is a common coordinate system used in MERRA-2, this coordinate system uses the independent variable to represent a scaled pressure level between the surface and 0.01 hPa. MERRA-2 analysis data are computed on a latitude–longitude cubed sphere grid at the same spatial resolution as the 3DVAR algorithm atmospheric model based on the Gridpoint Statistical Interpolation (GSI). MERRA-2 provides a timely replacement for MERRA (which was created with GEOS-5.2.0). It was expanded to include more recent satellite data: the Infrared Atmospheric Sounding Interferometer (IASI), the Cross-Track Infrared Sounder (on the Suomi-NPP satellite), and Advanced Technology Microwave Sounder (also on Suomi-NPP satellite), geostationary radiances from MSG SEVIRI and Geostationary Operational Environmental Satellites (GOES-11, GOES-13, and GOES-15), temperature and ozone profiles from EOS Aura MLS, wind speeds from the Meteorological Operational Satellite-A (MetOp-A) ASCAT and WindSat in addition to those already
used in the prior release of MERRA. Details of the model are described in Gelaro et al., (2017).

MERRA-2 includes the assimilation of aerosol data, which provides a multidecadal reanalysis in which aerosol and meteorological observations are jointly assimilated within a global data system (Gelaro et al., 2017). The MERRA-2 aerosol analysis system provides fundamental variables for this study, specifically the 3-hourly MERRA-2 assimilated aerosol output (MERRA-2 inst3_3d_aer_Nv: 3d, 3-Hourly, Instantaneous, Model-Level, Assimilation, Aerosol Mixing Ratio) and 1-hourly dust scattering AOD (MERRA-2 tavg1_2d_aer_Nx: 2d, 1-Hourly, Time-averaged, Single-Level, Assimilation, Aerosol Diagnostics) on the native 72 layers (GMAO, 2015a). The AOD observations are derived from several sources, including Level-2b 630 and 860 nm channels clear-sky radiance from AVHRR, reflectance from MODIS from the 0.66, 0.86, 0.47, 0.55, 1.24, 1.64 and 2.12 µm channels on Terra and Aqua, AOD retrievals from Multi-angle Imaging SpectroRadiometer (MISR) and the ground-based Aerosol Robotic NETwork (AERONET) AOD measurements. MERRA-2 includes three-dimensional mass mixing ratios of five-aerosol species as prognostic aerosol tracers depending on the size of the aerosol. Table 3 outlines the details of MERRA-2 data needed as input to the model simulations.

Figures 10 and Figure 11 plots the SST and AOD coverage of a dust outbreak season during Aug 18, 2017. This research will use 12 noon of this day's data for the model simulations, because the outbreak is relatively strong at this time.
Table 3. MERRA-2 data used in this study

<table>
<thead>
<tr>
<th>Data Name</th>
<th>Variable</th>
<th>Spatial resolution</th>
<th>Time resolution</th>
</tr>
</thead>
<tbody>
<tr>
<td>inst1_2d_asm</td>
<td>2m Temperature 2m Specific Humidity Sea Surface Temperature 10m V (northward wind) 10m U (eastward wind)</td>
<td></td>
<td>1-hourly</td>
</tr>
<tr>
<td>inst3_3d_aer_Nv</td>
<td>Dust Mixing Ratios at each layer</td>
<td>0.5°*0.625°</td>
<td>3-hourly</td>
</tr>
<tr>
<td>inst3_3d_asm_Nv</td>
<td>Air temperature Specific humidity Relative humidity</td>
<td></td>
<td>3-hourly</td>
</tr>
<tr>
<td>tavg1_2d_aer_Nx</td>
<td>Dust scattering AOD at 550 nm</td>
<td></td>
<td>1-hourly</td>
</tr>
<tr>
<td>tavg1_2d_rad_Nx</td>
<td>Total Cloud Area Fraction</td>
<td></td>
<td>1-hourly</td>
</tr>
</tbody>
</table>

Figure 10. MERRA-2 input SST data during a dust break on Aug.18 2017.

Figure 11. MERRA-2 input AOD data during a dust break on Aug.18 2017.
Chapter 4 Technical Approach and Methodology

Our goal is to better understand the characteristics and physical mechanisms of the aerosol layer effects on satellite retrieved IR $SST_{\text{skin}}$, and to derive an empirical formula that leads to improved corrections for the aerosol-related effect. The goal can be divided into seven main objectives; the specific steps to reach each main objective are then described:

a. Preprocess the data: collocate satellite data and model data with the in-situ measurements.

b. Apply quality control and generate match-ups.

c. Evaluate the accuracy of satellite $SST_{\text{skin}}$. Assess the impact of aerosol on satellite retrieved $SST_{\text{skin}}$.

d. Use Radiative transfer models (RTTOV) to simulate the $SST_{\text{skin}}$ differences with aerosol optical depth (AOD) and derive the Dust-introduced SST Difference Index (DSDI) based on ancillary data from MERRA-2.

e. Use 80% of the Match-up database (MUDB) to obtain coefficients for the DSDI algorithm.

f. Apply the new algorithm to this region, compare the new, aerosol corrected $SST_{\text{skin}}$ with in-situ SST.

g. Use the remaining 20% of the data to validate this approach.

An empirical correction formula will be derived, the flow diagram of our method is shown in Figure 12.
Figure 12. Analysis flow diagram.
4.1 Dust spectral optical properties

The calculation of dust spectral optical properties is based on the Lorentz-Mie scattering calculation using recent data on region-specific index coefficients and in situ measurement of particle size distribution of regional dust outflow over oceans based on OPAC (Optical Properties of Aerosols and Clouds) model and the dust optical properties by Claudia Di Biagio et al. (2017). The long-wave (LW) complex refractive index \( m \) of different dust aerosol, water vapor and fog based on simultaneous measurements of the particle was retrieved.

\[
m = n - ik
\]

*Equation 13*

\( n \) is the refractive index and \( k \) is the extinction coefficient. According to electromagnetic theory, \( n \) and \( k \) must satisfy the Kramers–Kronig (K–K) relationship (Bohren and Huffman, 1983):

\[
n(\omega) - 1 = \frac{2}{\pi} P \int_0^\infty \frac{\Omega * k(\Omega)}{\Omega^2 - \omega^2} d\Omega
\]

*Equation 14*

\( \omega \) is the angular frequency of radiation and \( P \) is the principal value of the Cauchy integral. \( n \) and \( k \) can be written as a function of the real \( \varepsilon_r(\omega) \) and imaginary \( \varepsilon_i(\omega) \) parts of the particle dielectric function:

\[
n(\omega) - 1 = \left(\frac{1}{2} \left[ \varepsilon_r(\omega)^2 + \varepsilon_i(\omega)^2 + \varepsilon_r(\omega) \right] \right)^{1/2}
\]

\[
k(\omega) - 1 = \left(\frac{1}{2} \left[ \varepsilon_r(\omega)^2 + \varepsilon_i(\omega)^2 - \varepsilon_r(\omega) \right] \right)^{1/2}
\]

*Equation 15*
furthermore, real $\varepsilon_r(\omega)$ and imaginary $\varepsilon_i(\omega)$ parts can be expressed as the sum of N Lorentzian harmonic oscillators:

$$\varepsilon_r(\omega) = \varepsilon_\infty + \sum_{j=1}^{N} \frac{F_j (\omega_j^2 - \omega^2)}{(\omega_j^2 - \omega^2)^2 + \gamma_j^2 \omega^2}$$

$$\varepsilon_i(\omega) = \sum_{j=1}^{N} \frac{F_j \gamma_j \omega}{(\omega_j^2 - \omega^2)^2 + \gamma_j^2 \omega^2}$$

Equation 16

$\varepsilon_\infty = n_{vis}^2$ is the real dielectric function in the limit of visible wavelengths, $n_{vis}$ is the real part of the refractive index in the visible, $F_j$, $\omega_j$ and $\gamma_j$ are strength respectively, eigenfrequency and damping factor characterizing the jth oscillator (Biagio et al. 2017).

Figure 13. Real and imaginary parts of the refractive indices of different particle optical properties are given for each wavelength. (Hess et al. 1998). Four gray stripes in the background means MODIS AQUA infrared channels 20 ($\lambda=3.8 \ \mu m$), 29 ($\lambda=8.9 \ \mu m$), 31 ($\lambda=11 \ \mu m$), 32 ($\lambda=12 \ \mu m$).

The OPAC database describes the microphysical and optical properties of six types of water clouds, three ice clouds, and ten aerosol components (Hess et al. 1998). Figure 13 shows the impact of various particle properties on the spectral features, we simulate the brightness temperatures of MODIS AQUA infrared channels 20 ($\lambda=3.8 \ \mu m$),
29 ($\lambda=8.9$ μm), 31 ($\lambda=11$ μm), 32 ($\lambda=12$ μm) shown as the four gray stripes in Figure 13. We define brightness at $\lambda=11$ μm as BT$_{11}$ etc. Compared to water, sea salt and fog, the mineral-transported dust has opposite spectral behavior near MODIS channels 20, 29, 31 and 32. Then derived an aerosol index with the combination of simulated BT difference of different wavelength as BT$_{3.8}$-BT$_{12}$, BT$_{3.8}$-BT$_{8.9}$ and BT$_{11}$-BT$_{12}$.

Figure 14. Real part LW refractive index of dust by Di Biagio et al. 2017, the magnitude is observed to vary region to region, and the water refractive index is different from aerosol dust near some spectral range.

Figure 15. Imaginary part of LW refractive index of dust by Di Biagio et al. 2017. The magnitude of dust refractive index is observed to vary region to region, and the water refractive index is different from aerosol dust near some spectral range.
Di Biagio et al. (2017) computed refractive indices of dust from different in situ source regions in a large smog chamber. They generated different kinds of dust aerosols from 19 soils of 8 regions. They used a large smog chamber to re-suspend the aerosol samples from soils and their dataset provides the long-wave extinction spectra, size distribution and mineralogical composition. Figure 14 shows the real part (refractive index $n$) and Figure 15 shows the imaginary part (extinction coefficient $k$) of the particle refractive index. Because the Saharan Dust outflow area is our region of interest, in here we just plot the dust refractive indices for dust from Tunisia, Morocco, Algeria and Mauritania. Results from these two figures show that the real ($n$) and imaginary ($k$) LW refractive index of dust varies both in magnitude and spectral shape for dust from different source regions; the dust refractive index trend looks similar but dust has different spectral behavior compared to water vapor and fog, especially for the extinction coefficient parts at the wavelengths of interest.

For the 11μm and 12 μm channels, the water vapor extinction coefficient of cloud droplets is strong, which is the reason why the cloud-affected matchups are removed from our research. The water vapor extinction coefficient is higher than that of dust aerosol near the 3 μm channel, which means the aerosol effects are more easily detectable than in the 11 and 12 μm channels and the difference between these channels are useful for us to derive an index for aerosol but only at night. The imaginary parts of the refractive indices of dust are higher in band 31 than in band 32, so the difference between 11 and 12 μm channels can be used to differentiate dust from other components. When the difference between 11 and 12 μm channels value pixel is greater than zero, there is a high probability that the pixel indicates dust (Ackerman, 1997; Baddock et al., 2009).
The difference between the band 20 (λ=3.8 μm) and band 29 (λ=8.9 μm) can also indicate dust density. The higher the dust density, the larger the difference between 3.8 and 8.9 μm channels will be.

4.2 RTTOV simulations

The effect of dust aerosols on MODIS retrieved SST_{skin} can be simulated using a multiple scattering radiative transfer model. RTTOV is a fast-radiative transfer model that simulates satellite observations for a number of passive infrared and microwave satellite instruments viewing the atmosphere and surface, such as MODIS, AVHRR, SEVIRI (Vidot, 2015). It also combines Line-by-Line Radiative Transfer Model (LBLRTM). RTTOV is developed by the EUMETSAT Numerical Weather Prediction Satellite Application Facility (NWP-SAF, https://www.nwpsaf.eu/site/software/rttov/). Here we use version 12.1 of RTTOV which is the most recent version.

The RTTOV performs a multivariate Taylor expansion of the formulation of the transmittance ratio between two adjacent layers (Vidot, 2015). The absorption optical depth in a channel i from TOA to level j can be predicted as:

\[
\tau_{a,i,j} = \tau_{a,i,j-1} + \sum_{k=1}^{K} (c_{i,j,k}X_{i,k})
\]

Equation 17

where \( c \) are the coefficients and \( X \) are the predictors (with total K values). Predictors are functions of atmospheric variables (pressure, temperature, absorber amount) and secant of the zenith angle of propagation.
RTTOV uses the Equation 18, derived from Equation 12, to calculate the integral transmittance parameters of each layer. Equation 18 represents the surface of earth and atmosphere’s radiance:

\[ R_{clr}(\lambda, \theta) = \varepsilon(\lambda, \theta)B(T, \lambda)\tau_{sfc}(\lambda, \theta) + \int_{\tau_{sfc}}^{1} B(T, \lambda)d\tau + \int_{\tau_{sfc}}^{1} [1 - \varepsilon_{sfc}(\lambda, \theta)]\int_{\tau_{tot}}^{1} \frac{B(T, \lambda)}{\tau_{tot}^2}d\tau \]

\textit{Equation 18}

where the transmittances \( \tau \) are calculated by regression of the input profile optical depth.

\begin{figure}
\centering
\includegraphics[width=\textwidth]{aerosols_desert_tropical_profile.png}
\caption{The radiative impact of the Continental Clean aerosol type (black curve) and the error introduced by the scaling approximation (red curve) for the tropical profile for two different aerosol number densities (Matricardi, 2015).}
\end{figure}

The Saharan desert aerosol type has significant impact on the detected radiance. Figure 16 shows that for the extreme condition case the presence of desert dust in a
tropical profile can result in a reduction of the top of the atmosphere radiance by 4K in the thermal infrared and by 1.8K in the mid-infrared by changing the aerosol number density from the background to 4x background (Matricardi, 2005). The desert dust aerosol type introduced larger effect on TOA BTs than other aerosol types. BT simulations for MODIS AQUA infrared channels 20 (3.8 μm), 29 (8.6 μm), 31 (10.8 μm), 32 (12 μm) have been performed with the RTTOV model.

Surface pressures are set to 1013 hPa and top of atmospheric pressure is 0 hPa. The atmosphere is divided into 54 layers, for which the atmospheric gas transmission coefficients are provided by RTTOV. Satellite zenith angle values are between 0° to 72°. The TOA radiances simulation including aerosols, RTTOV has employs ten aerosol components and a volcanic ash component. Many specific aerosol types can be simulated by mixing these 11 components. For the input aerosol profiles, OPAC model defined "Mineral Transported" type to do the simulations were used. The particle concentrations correspond to MERRA-2 dust mixing ratio data based on Vidot (2015).

Table 4. Mineral transported aerosol type and layer depth.

<table>
<thead>
<tr>
<th>Layer depth</th>
<th>Pressure Layer</th>
</tr>
</thead>
<tbody>
<tr>
<td>0-1km</td>
<td>1013hPa, 975hPa, 937hPa, 898hPa</td>
</tr>
<tr>
<td>1-2km</td>
<td>864hPa, 830hPa, 794hPa</td>
</tr>
<tr>
<td>2-3km</td>
<td>763hPa, 732hPa, 701hPa</td>
</tr>
<tr>
<td>3-5km</td>
<td>656hPa, 610hPa</td>
</tr>
</tbody>
</table>

The vertical distribution of aerosol influences the accuracy of infrared-derived SST_{skin}. From our studies, dust present at 1 km altitude, corresponding to the pressure
layer as shown in Table 4, the pressure layer is defined as this table in RTTOV. MERRA-2 includes three-dimensional mass mixing ratios of these five-aerosol species as prognostic aerosol tracers. However, the RTTOV aerosol unit is in number concentration instead of mass concentration (Vidot, 2017). The optical properties of aerosols in RTTOV are pre-calculated for one particle per cm\(^3\). The pre-calculated optical properties have to be multiplied by the aerosol number concentration to calculate the total optical properties of each layer. Figure 17 shows the MERRA-2 input value to RTTOV.

The conversion term between mass concentration and number of concentration, called \( M_i^* \) (in gm\(^{-3}\)/cm\(^3\)), is provided for each OPAC aerosol types. (Hess, et al., 1998).

The conversion of the mass mixing ratio \( q_i \) of aerosol in number of concentration \( N_i \) is given by:

\[
N_i = q_i \frac{10^2 P}{R_{\text{moist}} T M_i^*}
\]

*Equation 19*

Where \( q_i \) is the mixing ratio from MERRA-2 for RTTOV aerosol type i, \( P \) is the atmospheric pressure in hPa, \( T \) is the atmospheric temperature in K. \( R_{\text{moist}} \) is the moist air gas constant in Jg\(^{-1}\)K\(^{-1}\) given by this equation:

\[
R_{\text{moist}} = R_{\text{dry}} (1 + \frac{1 - \sigma}{\sigma} q_{\text{H}_2\text{O}})
\]

*Equation 20*

The coefficient \( \sigma \) is given by:

\[
\sigma = \frac{M_{\text{H}_2\text{O}}}{M_{\text{dry}}}
\]

*Equation 21*

The gas constant for dry air is given by:
\[ R_{dry} = \frac{R}{M_{dry}} \]

*Equation 22*

\[ M_{dry} = 10^3 \frac{\rho_{dry}}{n_{dry}} \]

*Equation 23*

Where \( R \) is the ideal gas constant equal to 8.3144598 Jmol\(^{-1}\)K\(^{-1}\), \( M_{dry} \) is the mean dry air molar mass equal to 28.9644 g mol\(^{-1}\), \( M_{H_2O} \) is the water mole mass equal to 18.01528 g mol\(^{-1}\).

The value of \( M_i^* \) can be obtained from the OPAC model for our "Mineral Transported" type as:

\[ M_i^* = 1.59 \times 10^{-5} \text{ gm}^3/\text{ cm}^3 \]

<table>
<thead>
<tr>
<th>MERRA2 Input</th>
<th>RTTOV</th>
</tr>
</thead>
<tbody>
<tr>
<td>2m T 2m Q</td>
<td>1 km aerosol layer at different bottom pressure levels</td>
</tr>
<tr>
<td>Sea Surface Temperature 10m V 10m U</td>
<td>Mineral aerosol type</td>
</tr>
<tr>
<td>Dust Mixing Ratios at each layer as kg/kg</td>
<td>Surface Pressure as 1013hPa</td>
</tr>
<tr>
<td>Air temperature</td>
<td>Aerosol concentration</td>
</tr>
<tr>
<td>Specific humidity</td>
<td></td>
</tr>
<tr>
<td>Relative humidity</td>
<td>51 Layer data</td>
</tr>
<tr>
<td>Dust scattering AOD at 550nm</td>
<td></td>
</tr>
<tr>
<td>72 Layer data</td>
<td></td>
</tr>
</tbody>
</table>

*Figure 17. MERRA-2 input values of RTTOV*
4.3 Match-up summary

The goal of this section is to assess the accuracy of various satellite SST products by comparing them with in situ temperature measurements to explore various dependences of the bias errors, including aerosol effects. In this study, ‘match-up’ stands for a data vector that consists of a MODIS or SEVIRI SST\textsubscript{skin}, the brightness temperatures in the relevant spectral bands, times and locations of the measurements, and other data including from MERRA-2, and in-situ drifting buoy and M-AERI SST\textsubscript{skin}. The match-ups were collected where the distance of in situ measurement to the nearest clear-sky pixel is less than 10 km, and the time difference between the satellite and in-situ data is less than 30 minutes (Kilpatrick et al, 2015). All satellite SST\textsubscript{skin} and BT are referenced to a 3x3 pixel extraction box centered on the position of the in situ measurement (Kilpatrick et al, 2015). For MODIS, the quality flag values can reflect the cloud cover. A smaller value means less chance of cloud contamination (0 is the best quality, 5 is worst quality). All MODIS SST products contain a numeric Quality Level for each pixel, assigned by evaluating test results, with quality level 0 being the highest quality and quality 4 being the worst. For SEVIRI, quality level 5 means the best quality data. Here, the MODIS SST pixels with quality flag values of 0, 1, 2 and SEVIRI SST pixels with quality flag values of 4, 5 are used.

In the context we define the satellite SST\textsubscript{skin} retrieval accuracy as the SST difference, $\Delta$SST, between the derived satellite SST\textsubscript{skin} ($\text{SST}_{\text{satellite}}$) and the in-situ skin SST ($\text{SST}_{\text{in-situ}}$):

$$\Delta \text{SST} = \text{SST}_{\text{satellite}} - \text{SST}_{\text{in-situ}}$$

\textit{Equation 24}
The Saharan outflow region can be defined as the area between 20°S and 35°N, and between 90°W and 90°E. The polar orbiting satellites pass each station location twice a day, once during the day and again at night. After match-up with in-situ SST and filtering of cloud contaminated data, the Version 6 MODIS SST\textsubscript{skin} processing algorithm night data have a mean error of –0.494°C, which is a large error compared to the global estimates as shown in Minnett et al. 2016. The accuracy of MODIS SST\textsubscript{skin} is poorer when validated against in situ SST from the Saharan Outflow area, with a mean error of –0.772°C. This may be due to the effects of the aerosols and the dry layer on infrared SST\textsubscript{skin}. Another possible cause for the errors of MODIS SST\textsubscript{skin} over the Saharan outflow area is that the high concentration of water vapor in the tropical ocean, results in a smaller component of the signal received at the satellite having originated from the ocean. The errors in this latitude band away from Saharan outflow are relatively small, which means the errors of MODIS SST\textsubscript{skin} over the Saharan outflow area is mainly caused by aerosol. Because of the flow divergence near the equator, drifting buoys tend to go towards the central ocean gyres (Lumpkin et al., 2012) leading to a relatively small number of match-ups. The MODIS Aqua SST Difference near Saharan Outflow area as shown in Figure 18.

This research has used the Aqua and CALIPSO aerosol data in these analyses. Aerosol effects on Aqua MODIS SST\textsubscript{skin} have been studied for 2015 using 4223 data pairs with Aqua AOD. Because CALIOP is a nadir-looking LIDAR instrument which measures the power backscattered by particles in the atmosphere, the data are only along the ground track of the satellite, so we obtained only 1512 matchup points with CALIPSO in the Saharan outflow area. CALIPSO and Aqua observe the same target
within 2 min because they belong to same "A-Train" satellite constellation and CALIPSO just lags Aqua by 1 to 2 minutes.

![Difference between Aqua MODIS SST with in-situ drifting buoys SST](image)

Figure 18. MODIS Aqua SST Difference near Saharan Outflow area, the quality flag values of MODIS Aqua are 0, 1, 2.

**4.4 SEVIRI error distribution**

![SEVIRI(Satellite) with MAERI(in-situ) data](image)

Figure 19. SEVIRI and MAERI data; the x-axis is the time values of the SEVIRI MUDB. The SEVIRI and MAERI agree well and the SST difference is between ±2K. The histogram is the SST difference that grouped into bins of every 1K difference, the MAERI derived SST is cooler than M-AERI SST as shown in the histogram.
The match-ups were also collected for SEVIRI as shown in Figure 19. The SEVIRI data agrees well with MAERI, and it has a mean discrepancy when compared to M-AERI of −0.46°C and standard deviation of -0.59°C. The geographical distribution of the SST difference between SEVIRI and M-AERI to assess the impacts of the presence of aerosol layers is plotted in Figure 20. The regions where are expected aerosol layers to exist have significant errors in the retrieved SSTs in comparison to the errors found in the analyses of other aerosol-free ocean areas.

Figure 20. SEVIRI SST difference distribution with the track of ship. The color means the difference between SEVIRI SST and M-AERI SSTskin. The red boxes are Saharan Dust outbreak area, there are significant negative SST difference between them in this area.
4.5 MODIS differences with AOD

![SST Difference with AOD](image)

Figure 21. SST differences (MODIS SST\textsubscript{skin} between in-situ buoy SST) with MODIS Aerosol Optical Depth. This scatter plot is colored by the density of points. The red line is the fitted line of these points.

Table 5. Statistics of errors of MODIS Aqua SST vs in-situ measurements. The mean SST bias increases with AOD. Especially when AOD>0.5, the mean SST bias can be larger than 1K as marked as red color in this table.

<table>
<thead>
<tr>
<th>MODIS AOD</th>
<th>For the 2015 Match-up data ( K )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>N</td>
</tr>
<tr>
<td>0-0.2</td>
<td>3079</td>
</tr>
<tr>
<td>0.2-0.4</td>
<td>775</td>
</tr>
<tr>
<td>0.4-0.6</td>
<td>253</td>
</tr>
<tr>
<td>0.6-0.8</td>
<td>78</td>
</tr>
<tr>
<td>&gt;0.8</td>
<td>38</td>
</tr>
<tr>
<td>Total</td>
<td>4223</td>
</tr>
</tbody>
</table>
In the Saharan Outflow region, the $\text{SST}_{\text{skin}}$ difference has a negative relationship with AOD, as expected in Figure 21. From the statistics of errors between MODIS and in-situ SST (Table 5), when the AOD is less than 0.4, the mean difference between satellite and in-situ SST is within 0.7°C. At larger AOD, the effect of aerosols is more pronounced. This indicates the aerosol layers are major sources of residual errors in the derived $\text{SST}_{\text{skin}}$. The matchup data regression line fitted to the data has a slope of -1.90. Thus, there is a negative correlation between the $\text{SST}_{\text{skin}}$ differences and AOD.

![Column Integrated Attenuated Backscatter with Aerosol Layers](image)

*Figure 22. Column Integrated Attenuated Backscatter with Aerosol Optical Depth, the fitted red line clearly shows the aerosol in the atmosphere will attenuate backscatter signal.*
Figure 23. MODIS SST$_{skin}$ Difference with Layer Altitudes (Left: Top Altitude. Right: Base Altitude).

Figure 24. SST Difference with Number of Aerosol Layers. The SST difference increases with number of aerosol layers. The fitted red line shows the SST difference will be more negative with increasing of number of aerosol layers.
The LIDAR column integrated attenuated backscatter data with AOD data is plotted as in Figure 22, it is clear that the increase of aerosol particles in the atmosphere attenuates the backscatter signal.

The vertical distribution of aerosol influences the accuracy of infrared-derived SST$_{\text{skin}}$. From our studies, dust present at lower altitudes has a smaller effect on the SST$_{\text{skin}}$ errors (Figure 23). Compared with layer base altitude, the error is more sensitive to the layer top altitude, because the higher dust layers have a greater temperature difference compared to the sea surface. Furthermore, the relationship in Figure 24 shows the SST$_{\text{skin}}$ difference is also related to the number of aerosol layers.

The error in SST$_{\text{skin}}$ is more sensitive to the altitude of the top of the aerosol layer than the bottom of the layer as the temperature difference between the top of the dust layer and the sea surface is typically larger.
4.6 SEVIRI differences with AOD

Figure 25. SEVIRI differences with respect to M-AERI with AOD, the SST difference increases with AOD.

Figure 26. SEVIRI differences with AOD. The left Y-axis means the MODIS SST minus in-situ measurement SST, the right Y-axis means the MODIS derived AOD. As shown in the green ovals, when there is large AOD, the strong aerosol in the atmosphere causes more negative SST difference.
Figure 27. SEVIRI SST differences respected with ECMWF with AOD. Left is the SST difference between ECMWF model data and SEVIRI SST data, there is negative bias near Sahara outflow area as shown in right figure where the AOD is relatively high. The MODIS AOD daily sampling data offered here have large data gaps due to presence of clouds and the path of the Aqua satellite.

Table 6. Statistics of errors of Meteosat SEVIRI SST vs AOD

<table>
<thead>
<tr>
<th>MODIS AOD</th>
<th>Between the 2006/2007/2008/2011/2015 M-AERI with SEVIRI data</th>
<th>N</th>
<th>Min</th>
<th>Max</th>
<th>Median</th>
<th>Mean</th>
<th>STD</th>
</tr>
</thead>
<tbody>
<tr>
<td>0-0.2</td>
<td></td>
<td>1844</td>
<td>-1.734</td>
<td>2.908</td>
<td>-0.022</td>
<td>-0.025</td>
<td>0.502</td>
</tr>
<tr>
<td>0.2-0.4</td>
<td></td>
<td>1392</td>
<td>-2.787</td>
<td>1.483</td>
<td>-0.392</td>
<td>-0.429</td>
<td>0.545</td>
</tr>
<tr>
<td>0.4-0.6</td>
<td></td>
<td>576</td>
<td>-2.653</td>
<td>0.168</td>
<td>-0.891</td>
<td>-0.916</td>
<td>0.462</td>
</tr>
<tr>
<td>0.6-0.8</td>
<td></td>
<td>178</td>
<td>-2.925</td>
<td>0.192</td>
<td>-0.978</td>
<td>-1.052</td>
<td>0.629</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td>4108</td>
<td>-2.925</td>
<td>2.908</td>
<td>0.285</td>
<td>-0.356</td>
<td>0.636</td>
</tr>
</tbody>
</table>

The SEVIRI SST<sub>skin</sub> with the in-situ M-AERI SST<sub>skin</sub> data have mean differences of -0.356K and standard deviation of 0.636K. The largest negative SEVIRI-MAERI
differences are in the Saharan outflow area where satellite SST retrievals are challenging and under the influence of dust. The degree of statistical significance of the difference of each match-up dataset was evaluated using MODIS Aerosol Optical Depth data assuming that all match-ups have independent errors. There are 4108 data pairs with Aqua AOD and their relation is plot in figure 25. Figure 26 shows MODIS AOD and the SST difference of the SEVIRI. It is clear that the difference between them is correlated with the aerosol layers. SEVIRI SST_{skin} algorithms are also sensitive to dust layer, when AOD is > 0.5, the SST_{skin} has ~1 K difference. Figure 27 shows the SEVIRI SST differences respected with ECMWF with MODIS derived AOD. The negative SST bias region corresponds to high AOD region, which means the aerosol will have negative difference for infrared satellite.
Chapter 5 Results

This chapter outlines the model simulation results and application of this empirical correction formula to MODIS SST_{skin} data. The first section describes the RTTOV simulations of dust effect; this research uses these simulations to derive the Dust-introduced SST Difference Index (DSDI) formula. This is followed by an outline of the simulations of Satellite Zenith Angle dependence of the DSDI. Then we apply this method to MODIS MUDB and the new DSDI coefficients are derived by regressions on the MODIS BT difference and SST_{skin} difference. The last section validates this approach to give insight as to how the empirical formula operates. Errors are characterized and analyzed in this section.

5.1 RTTOV model simulation of aerosol dust

The effect of dust aerosols on MODIS retrieved SST_{skin} can be simulated using a multiple scattering radiative transfer model. The Saharan Desert aerosol type has significant impact on the top-of-atmosphere (TOA) radiance.

Merchant et al. (2006) used the Hess et al. (1998) and Highwood et al. (2003) aerosol properties to plot the BT change against 10 μm AOD for four channels of SEVIRI. From their model simulations, they predicted not only changes in the BTs due to the presence of desert dust, but also changes in the BT differences as shown in Figure 28. They defined the SEVIRI Saharan Dust Index (SDI), using second principal component of the brightness-temperature difference space. The off-axis characteristic was empirically found to be linearly related to Saharan-Dust affected BTs in observations. Then they used
the relationship between SST\textsubscript{skin} bias and SDI to correct the algorithms, which reduced SST\textsubscript{skin} errors to +0.20 K.

Following the approach of Merchant et al. (2006) in developing the SEVIRI SDI as shown in Figure 28, the newest version of RTTOV 12.1 is used to simulate top of atmosphere BTs for conditions that include various dust layers. Aerosol effects on the TOA BTs increase with increasing dust altitude, as was shown in Section 4.5 and Figure 23.

*Figure 28. Changes in BT difference versus AOD assuming a layer of aerosol evenly distributed between 2 and 3 km altitude. (a) and (b) use Haywood optical properties. (c) and (d) use OPAC dust parameters. (Merchant et al. 2006).*
Figure 29 and Figure 30 show the simulated MODIS BT difference between wavelengths 11 μm and 12 μm, 3.8 μm and 12 μm, 3.8 μm and 11 μm, and 3.8 μm and 8.9 μm as a function of Aerosol Concentrations.

**Figure 29.** Changes in BT difference versus Aerosol Concentrations. With the increasing of the aerosol concentrations, the BT difference between different channels will decrease or increase. This characteristic can be used to deduce the DSDI formula.

**Figure 30.** BT difference with SST skin difference, the color indicate different values of aerosol related SST skin differences.
The model was run for prescribed MERRA-2 atmospheric and surface conditions, together with input dust mixing ratios and aerosol distributions. The distribution and concentration of aerosols have an effect on the simulated SST differences as found in previous studies. From our research, the change in BT is not linear with AOD as was shown by Merchant et al. (2006) in Figure 28.

Furthermore, BT$_{11}$- BT$_{12}$, BT$_{3.8}$- BT$_{12}$, BT$_{3.8}$-BT$_{8.9}$ are more useful to derive the DSDI. This research examined the SST$_{skin}$ difference versus BT difference and derived the new-version MODIS Aqua Dust-introduced SST Difference Index (DSDI) using:

$$DSDI= a_0+a_1*(BT_{3.8}-BT_{12}) + a_2*(BT_{3.8}-BT_{8.9}) + a_3 *(BT_{11}-BT_{12}) + a_4 *(BT_{11}-BT_{12})^2$$

*Equation 25*

where $a_0 =0.477$  $a_1 =0.234$  $a_2 =0.125$  $a_3 =-0.474$  $a_4 =0.025$

The model can be run with aerosol and without the aerosol to derive the SST$_{skin}$ difference. The coefficients are derived by regressions of the BT difference and SST$_{skin}$ difference using the RTTOV model simulations.

![Image](image.png)

*Figure 31. Derived DSDI and its relationship with SST$_{skin}$ difference and aerosol concentration. The left figure clearly shows the aerosol layer causes negative SST difference and the right figure shows how DSDI is related to the aerosol layer and can be used to correct the SST$_{skin}$ difference.*
Figure 32. Difference in simulated $SST_{\text{skin}}$ when aerosols are present or not. The $SST_{\text{skin}}$ difference is related to the aerosol distribution.

There is a clear connection between $SST_{\text{skin}}$ difference and DSDI as shown in Figure 31 and Figure 32; the $SST_{\text{skin}}$ difference decrease nearly linearly with DSDI. From scatter plot of the DSDI distributions as shown in Figure 33, it can demonstrate that the DSDI can capture the $SST_{\text{skin}}$ difference variability due to the Saharan Dust layer. DSDI equation derived from simulations can be used to correct the $SST_{\text{skin}}$ retrievals. It needs to be clarified that this DSDI is just an index which indicates how much the observed BTs have deviated from typical clear-sky conditions (Merchant et al. 2006, Le Borgne et al., 2013).

Figure 33. Derived Dust-introduced SST Difference Index. Compared to Figure 29, the derived DSDI distribution is clearly related to the $SST_{\text{skin}}$ difference.
5.2 RTTOV model simulation of satellite zenith angle

Satellite Zenith Angle is the angle between a straight line from a point on the earth's surface to the satellite and a line from the same point on the earth's surface that is perpendicular to the earth's surface at that point (the zenith point). (https://definedterm.com/satellite_zenith_angle), as defined in Figure 34. From the match-up database in NOAA iQuam (Ignatov et al 2016), we can also find that the SST night time bias between these two datasets is greater when the satellite view angle is above 60° as shown in Figure 35.
Figure 35. SST Difference with satellite view angle (Ignatov et al 2016). The data that are used are from NOAA16, NOAA17, NOAA18, NOAA19 and METOPA satellite, the y-axis is the SST difference between satellite and buoys.

Figure 36. RTTOV simulated SST\textsubscript{skin} difference as a function of Satellite Zenith Angle. Based on simulated 300 data points of nighttime BT at 36 view angles (0\(^\circ\) to 72\(^\circ\)) under aerosol-free conditions.

On average, increasing the AOD and the satellite zenith angle increase the SST\textsubscript{skin} difference, because the optical path length of the dust layer emission increases with satellite zenith angle \( \theta \). The SST\textsubscript{skin} error due to satellite zenith angle is a approximately cosine function as shown in Figure 36, which provides a useful method for an empirical
correction. Following Le Borgne et al. (2013) in developing the VIIRS SDI, we add the satellite zenith angle correction terms in our DSDI equation 25.

5.3 Derivation of a MODIS correction algorithm using MUDB

Encouraged by the RTTOV simulations, this research use the MODIS SST\textsubscript{skin} data in the MUDBs with quality levels of 0, 1 and 2 which represent both cloud free data, and some with cloud/aerosol contamination. Regression against in-situ data is used to determine the coefficients in the DSDI equation. Eq.26 represents the empirical DSDI for MODIS:

\[ \text{DSDI} = a_0 + a_1*(\text{BT}_{3.8} - \text{BT}_{12}) + a_2*(\text{BT}_{3.8} - \text{BT}_{8.9}) + a_3*(\text{BT}_{11} - \text{BT}_{12}) + a_4*(\text{BT}_{11} - \text{BT}_{12})^2 \]

\textit{Equation 26}

where \( a_0 = 0.533 \), \( a_1 = 0.475 \), \( a_2 = 0.207 \), \( a_3 = -1.985 \), \( a_4 = -0.113 \)

\[ \text{Figure 37. Left: scatter plot of the SST}_{\text{skin}} \text{ difference with BT}_{3.8} - \text{BT}_{12} \text{ and BT}_{11} - \text{BT}_{12}, \text{ color means the SST}_{\text{skin}} \text{ difference, it can be used to represent the aerosol introduced SST}_{\text{skin}} \text{ difference. Right: Derived DSDI with BT difference, corresponding to the left picture and it can be used to correct the SST}_{\text{skin}} \text{ difference.} \]
Figure 38. BT Difference with SST\textsubscript{skin} difference, this scatter plot takes the satellite view angle term \( S_0 \) into account. Color indicates SST\textsubscript{skin} difference. It can easily distinguish the SST\textsubscript{skin} difference using the BT difference after adding satellite view angle term.

Since the satellite zenith angle will cause SST\textsubscript{skin} error as a cosine function as discussed in Section 5.2 and discussed by Ignatov et al 2016 with IQUAM MUDB in Figure 35, we take the satellite zenith angle term into account and scatter plot the BT Difference with SST\textsubscript{skin} difference as shown in Figure 38, the new plot clearly shows the distinction of the color compared to Figure 37. So the satellite zenith angle correction term is also useful in our DSDI equation.

A new DSDI equation and coefficients, which are derived by regressions of the BT difference with a satellite zenith angle dependence and SST\textsubscript{skin} difference in the MUDBs, has been developed based on Equation 27:

\[
DSDI = a + (b + c*S_0) \times (\text{BT}_{3.8} - \text{BT}_{12}) + d \times (\text{BT}_{3.8} - \text{BT}_{8.9}) + (e + f*S_0) \times (\text{BT}_{11} - \text{BT}_{12}) + (g + h*S_0) \times (\text{BT}_{11} - \text{BT}_{12})^2
\]

\textit{Equation 27}

where \( a = 0.4246 \) \( b = 0.475 \) \( c = -0.1604 \) \( d = 0.207 \) \( e = -1.985 \) \( f = 0.351 \) \( g = -0.113 \) \( h = 0.060 \) and \( S_0 = \sec(\Theta) - 1 \).
The error analysis associated with this developed DSDI are shown in Table 7. I leave one out of the current terms systematically from Eq. 27, and reassess the fit and its mean errors, standard deviation (STD) and Root mean squared value (RMS) of remaining terms. After removing (BT_{3.8}-BT_{12}) or (BT_{11}-BT_{12}) term, the correlation between the new DSDI and the original DSDI is relatively small, at the same time the STD and RMS are large, which means these two terms are relatively important in derived DSDI. The (BT_{11}-BT_{12})^2 term has less effect on derived DSDI compared to other terms, but it is still important because (BT_{11}-BT_{12}) is not linearly with aerosol concentrations.

**Table 7 Error analysis associated with developed DSDI.**

<table>
<thead>
<tr>
<th>Leaving Terms</th>
<th>Remaining terms relation with DSDI (Eq. 27)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(b + c*S_0) * (BT_{3.8} - BT_{12})</td>
<td>Correlation  Mean  Median  STD  RMS</td>
</tr>
<tr>
<td></td>
<td>0.166 1.530 1.407 0.757 1.708</td>
</tr>
<tr>
<td>d * (BT_{3.8}-BT_{8.9})</td>
<td>0.547 0.986 0.962 0.272 1.023</td>
</tr>
<tr>
<td>(e + f*S_0) * (BT_{11}-BT_{12})</td>
<td>0.304 -2.409 -2.310 0.831 2.549</td>
</tr>
<tr>
<td>(g + h*S_0) * (BT_{11}-BT_{12})^2</td>
<td>0.914 -0.166 -0.133 0.119 0.204</td>
</tr>
</tbody>
</table>

**Figure 39. Distribution of empirically derived DSDI.** The DSDI value is relatively high in the Saharan dust outbreak area. In other words, the DSDI can be used to represent the SST difference with respect to drifter measurements and can be used to correct the MODIS SST_{skin} retrieval algorithms.
Table 7 can demonstrate how much information each additional term is contributing to DSDI. The distribution of DSDI also corresponds to Saharan aerosol dust area as shown in Figure 39. Figure 40 shows the relationship between MODIS SST\text{skin} difference with In-situ measurements and DSDI, indicating there is a high correlation between them.

![SST Difference with Dust-introduced SST Difference Index](image)

*Figure 40. Empirical derived DSDI with SST\text{skin} Difference.*

SST difference will be more negative with increasing of the DSDI, the aerosol introduced SST difference is usually > 1 K when DSDI > 0.8. The relationship between DSDI and SST difference is not clear when DSDI is < 0.8. Apply $DSDI > 0.8$ to select the conditions where the correction can be applied as shown in Figure 40. Then the new selected points are plotted in Figure 41.
Aerosol dust effect on SST difference becomes significant for the MODIS nighttime DSDI values above 0.8, and the DSDI is linearly related with SST difference when DSDI>0.8. After regressing the SST\textsubscript{skin} errors against DSDI, we obtain Eq.29 and use this formula to derive the Dust-introduced SST Difference Index correction (DSDI\textsubscript{Correction}) term. It could be added to the NLSST algorithm for correction of the aerosol-induced SST\textsubscript{skin} errors:

\[ \text{DSDI\textsubscript{Correction}} = 0.628 \times \text{DSDI}^2 - 4.528 \times \text{DSDI} + 2.071 \]

\textit{Equation 28}
Figure 42. Difference between Aqua MODIS SST with in-situ buoy SST before DSDI correction.

Figure 43. Difference between Aqua MODIS SST with in-situ buoy SST after correction.

Figure 44. The difference in $SST_{skin}$ between before and after aerosol correction. This aerosol correction term is high at Saharan dust outflow area.
Figure 45. Histograms of the SST\textsubscript{skin} difference, before and after correction. The mean SST difference has decreased by an amount of 0.18K. There are a few points below -2K after correction.

Figure 43 shows the effects of applying the DSDI correction term to the derived SST\textsubscript{skin} using the match-up database. Compared to Figure 42, the mean bias value has decreased by 0.18K. The difference between them are plotted in Figure 44. This aerosol correction term value is relative high near dust outflow region. Figure 45 shows the histograms of the SST\textsubscript{skin} difference before and after DSDI correction.

**Table 8. Error statistics according to MODIS quality flag**

<table>
<thead>
<tr>
<th>Quality Level</th>
<th>N</th>
<th>Before correction</th>
<th>After correction</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Mean</td>
<td>Median</td>
</tr>
<tr>
<td>0</td>
<td>86092</td>
<td>-0.217</td>
<td>-0.190</td>
</tr>
<tr>
<td>1</td>
<td>47030</td>
<td>-0.482</td>
<td>-0.435</td>
</tr>
<tr>
<td>2</td>
<td>50919</td>
<td>-0.974</td>
<td>-0.830</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td>184041</td>
<td>-0.494</td>
<td>-0.355</td>
</tr>
</tbody>
</table>

Table 8 shows the error statistics at different quality level. Compare to level 0 and level 1, there is much more benefit for level 2 data, the average increase for level 2 data is
0.296K. Thus, this correction method works well for the data that are usually recognized as poor quality, which means it can improve the fraction of useful data available instead of discarding the bad quality data.

This research uses a large area to calculate the aerosol effects on SST$_{skin}$ retrieval, so the decrease of bias and standard deviation is not so obvious. Selecting a smaller area (0°N to 25°N, 40°W to 10°E, shown in Figure 46), which area is more likely be affected by aerosol dust, from a Gaussian distribution of the SST bias (Figure 47), the SST$_{skin}$ bias and standard deviation can be reduced significantly by 0.26K and 0.15K.

![Figure 46. Before and after correction the SST difference. Because this area is near the Saharan dust outflow area and the satellite retrieved SST is more likely to be affected by the dust aerosol in this region.](image-url)
5.4 Validation of this approach

Table 9. Statistics of the difference between MODIS Aqua SST and in-situ temperature in this region (between 90° W to 90° E and 20° S to 35° N.)

<table>
<thead>
<tr>
<th>year</th>
<th>For the Matchup Data bases data</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Number of matchups</td>
<td>Mean (°C)</td>
</tr>
<tr>
<td>2010</td>
<td>32896</td>
<td>-0.516</td>
</tr>
<tr>
<td>2011</td>
<td>35946</td>
<td>-0.502</td>
</tr>
<tr>
<td>2012</td>
<td>29441</td>
<td>-0.509</td>
</tr>
<tr>
<td>2013</td>
<td>38637</td>
<td>-0.467</td>
</tr>
<tr>
<td>2014</td>
<td>14300</td>
<td>-0.460</td>
</tr>
<tr>
<td>2015</td>
<td>32821</td>
<td>-0.495</td>
</tr>
<tr>
<td>Total</td>
<td>184041</td>
<td>-0.494</td>
</tr>
</tbody>
</table>

Using RTTOV infrared radiative transfer modeling through the atmosphere with properties provided by MERRA-2, this research has found the effects of atmospheric aerosol layers on the accuracy of retrievals of SST_{skin} and developed the Dust-introduced SST Difference Index to correct infrared satellite SST_{skin} retrievals.
Validation of the MODIS Aqua retrievals of SST_{skin} is presented. All of the MODIS SSTs are compared to drifting buoy and M-AERI observations over the period 2010 to 2015. Due to the fact that the mean errors and standard deviation are evenly throughout these years as shown in Table 9, we need not worry about time dependence. This research randomly selected 80% of the data to derive the MODIS DSDI equation and selected another 20% of the data to verify the behavior of this empirical correction of the aerosol introduced SST differences. Unfortunately, the buoys have very relatively sparse coverage in this tropical area.

Figure 48. Dust-introduced SST Difference Index applied to 20% of the data that were withheld in the derivation of the DSDI form and of the coefficients.
Based on the 20% validation data, Figure 49 shows the distribution of MODIS satellite retrieval difference with respect to buoy temperature before correction with an average of -0.491K, and Figure 50 shows the difference after correction with an average of -0.379K. There is reduced bias between satellite derived SST\textsubscript{skin} and in-situ SST, and the relation between DSDI and SST difference shown in Figure 48 also indicates that the correction approach is beneficial.
Chapter 6 Summary and Future Work

The goal of this study was to improve the accuracy of satellite derived SST_{skin} in conditions contaminated by mineral dust aerosols, thus providing data to improve our understanding by reducing uncertainty in satellite-derived SST_{skin} needed in projections of climate change and in environmental science. Both Numerical Weather Prediction and ocean forecasting models need accurate SST input; furthermore, improved SSTs are also important for maritime safety, fisheries information, etc. SST is usually retrieved from infrared instruments using a non-linear function of the observed BTs, and they typically use cloud masks to remove cloudy and heavy aerosol-contaminated measurements. Few existing retrieval schemes have been characterized in terms of their sensitivity of aerosol such as Merchant et al. (2006). The research presented here shows infrared satellite SST_{skin} discrepancies with respect to in-situ measurements caused by aerosols. An empirical correction formula has been developed and applied in this study. Utilizing in-situ data, satellite data and a matchup approach, the characteristics and physical mechanisms of the aerosol layer effects on satellite retrieved infrared SST_{skin} have been revealed, as well as deriving an empirical formula that better corrects for aerosol-related effects. Simulation of the measured brightness temperatures using the RTTOV radiative transfer model was used in this study to explore the functional form of the aerosol correction. The correction formula has been shown to be beneficial when applied to infrared measurements of MODIS on the Aqua satellite.

So far, this research has only performed a simple regression analysis to establish a relationship between SST_{skin} differences and aerosol, there is a need to develop more
robust algorithms that could lead to a more useful correction for aerosol effects.

Suggested future research work includes:

a. The night-time aerosol correction algorithm developed here is mainly influenced by the 3.8μm channel BTs. Since these BTs are contaminated by scattered and reflected solar radiation during the day, a correction algorithm for day-time use based on 8.9μm channel BTs, should be developed.

b. The vertical distribution of aerosol influences the accuracy of infrared-derived SST skin. This study has shown dust present at lower altitudes has a smaller effect on the SST skin errors. Compared with layer base altitude, the error is more sensitive to the layer top altitude, because the higher dust layers have a more significant temperature difference compared to the sea surface.

Figure 51. RTTOV simulated effects show the altitude of the aerosol layer has an impact on the SST skin retrieval. Different colors indicate different altitudes of the dust layers. With the increasing of aerosol height, the SST difference is more negative.
RTTOV simulated dust layer effects at different heights as described in Section 4.2 have an impact on the satellite SST retrieval as shown in Figure 51. Is the large SST difference due to the aerosol scattering or the temperature of the dust layer? Because the temperature difference between the dust layers and the surface also has a substantial impact at SST retrievals as shown above.

Both AQUA and CALIPSO belong to the A-Train, CALIPSO being just 2 minutes behind AQUA. CALIPSO provides information about the vertical distribution of aerosol layers, so aerosol height data can be used to derive different coefficients in the correction algorithms. The impact of different kinds of aerosol layers should be further explored.

c. Such approaches as developed here can be applied to other well-calibrated infrared satellite radiometers such as Visible Infrared Imaging Radiometer Suite (VIIRS) on the Suomi-NPP and NOAA-20 satellites and others in the future.

The research presented here can be built on to contribute to our understanding of the radiative characteristics and effects of Saharan dust on the top of atmosphere infrared radiance measurements. Such research would lead to improving the accuracy and quality of satellite derived SSTs. The research presented here was focused on the Saharan dust outflow area, it is anticipated that the results will have applicability to a wider geographical range where dust aerosol appear. In achieving the primary objectives of extended research, algorithms would be developed to be applicable to other areas where there are significant contaminations of infrared measurements from earth observation satellites caused by aerosols to correct SST errors at other areas.
References


Matricardi, Marco. (2005). The Inclusion of Aerosols and Clouds in RTIASI, the ECMWF Fast Radiative Transfer Model for the Infrared Atmospheric Sounding Interferometer. ECMWF Tech. Memo.. 474. Available at https://pdfs.semanticscholar.org/a0c0/2906459fadca01c2e4c80916a9c99af23d06.pdf


