

**Infrared Satellite-Derived Sea Surface Skin Temperature Sensitivity to
Aerosol Vertical Distribution – Field Data Analysis and Model
Simulations**

Submitted to SPECIAL SECTION on the "Terra Mission - 20 Years of Science"

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1 **Abstract**

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3
4 Sea surface temperature is an Essential Climate Variable. The radiative impact of mineral
5 dust is one of the major contributors to inaccuracies in the satellite-retrieved sea surface
6 skin temperature (SST_{skin}). Different aerosol dust vertical distributions have varying
7 effects on the satellite-derived SST_{skin} . To further investigate the physical mechanisms of
8 aerosol effects on Terra MODerate-resolution Imaging Spectroradiometers (MODIS)
9 derived SST_{skin} , the aerosol radiative effects were studied with a field-data match-up
10 analysis and radiative transfer simulations. The field data are measurements of the SST_{skin}
11 derived from highly accurate ship-based infrared spectrometers vertical atmospheric
12 temperature and water vapor radiosonde profiles. The aerosol dust concentrations in
13 three-dimensions from the NASA Modern-Era Retrospective analysis for Research and
14 Applications, Version 2 have been used as input to radiative transfer simulations. Based
15 on the analysis of field data and simulations, we have empirically determined that the
16 sensitivity of the Terra MODIS retrieved SST_{skin} accuracies is related to 1) dust
17 concentration in the atmosphere, 2) the dust layer altitude, and 3) the dust layer
18 temperature. As the aerosol altitude increases, the effect on the SST_{skin} retrievals becomes
19 more negative in proportion to the temperature contrast with the sea surface. SST_{skin}
20 differences, satellite-derived - surface measurements, for a given aerosol layer optical
21 depth vary between -3 K and 1 K according to our match-up comparisons and radiative
22 transfer simulations.

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25 **1. Introduction**

26 Sea-surface temperature (SST) is a major governing factor in air-sea exchanges of
27 heat, moisture, gases and momentum; it also indicates surface circulation patterns in the
28 upper ocean. Infrared imaging radiometers on polar orbiting, earth-observation satellites
29 have provided measurements for the retrieval of SST for a half-century (Minnett et al.
30 2019). Starting with the High Resolution Infrared Radiometer (HRIR) on the NASA
31 satellite Nimbus-1 (Allison and Kennedy 1967; Smith et al. 1970) and through a series of
32 Advanced Very High Resolution Radiometers (AVHRR, Cracknell (1997)), satellite SST
33 retrievals have played a significant role in generating time series of quantitative estimates
34 of SST (Kilpatrick et al. 2001; Merchant et al. 2019; Reynolds and Smith 1994). TERRA
35 was launched in December 1999 with a descending (from north to south) equatorial
36 crossing local time of 10:30 a.m. \pm 5 minutes (Xiong et al. 2008a). TERRA was
37 developed to pair with another EOS (Earth Observing System) satellite – AQUA – which
38 was launched in May 2002 into an orbit with an ascending node (from south to north)
39 equatorial crossing local time of around 13:30 p.m. Both satellites carry several
40 instruments to investigate the Earth’s atmosphere and surface. Over the past twenty years,
41 the Moderate Resolution Imaging Spectroradiometer (MODIS; Esaias et al. (1998))
42 onboard TERRA has taken nearly continuous measurements for more than 108,000 orbits,
43 with an unprecedented spectral resolution, while sampling the Earth’s surface and
44 atmosphere. The missions of the AVHRR and MODIS are being extended in the USA by
45 the Visible Infrared Imaging Radiometer Suite (VIIRS; Schueler et al. (2013)) onboard
46 the Suomi-National Polar-orbiting Partnership satellite (S-NPP) and NOAA20, with
47 further VIIRS to be flown on future NOAA polar-orbiting satellites (Minnett et al. 2020).

48 Radiometers on European satellites, such as the Sea and Land Surface Temperature
49 Radiometer (SLSTR; Merchant (2012); Donlon et al. (2012)) and the METImage
50 (Schmüling et al. 2010; Wallner et al. 2017), will also extend the SST record from polar-
51 orbiting satellites. These, and other infrared satellite instruments have provided other
52 atmospheric and oceanic data for use in weather forecasting and in operational
53 oceanography, and for studying the climate system. These satellite missions and
54 applications will continue into the foreseeable future (Minnett et al. 2019).

55 Definitions of various kinds of SST were introduced by the Group for High
56 Resolution SST (GHRSSST; Donlon et al. (2007)) according to the thermal variability of
57 the upper ocean. The infrared radiometer derived temperature is usually characteristic of
58 a depth of less than 1 mm, determined by the emission depth of the infrared radiation
59 (Bertie and Lan 1996; Donlon et al. 2014b; Downing and Williams 1975; Hale and
60 Querry 1973; Judd and Handler 2019). During daytime the temperature variability is
61 influenced by absorbing solar radiation, modulated by cloud cover, as well as by losing
62 heat to the atmosphere, the latter being dependent on surface wind and surface-driven
63 turbulence and occurring during both daytime and nighttime (Gentemann et al. 2009;
64 Minnett 2003). More detailed discussions of near-surface SST are given by Donlon et al.
65 (2007) and Minnett and Kaiser-Weiss (2012).

66 Sea surface skin temperature (SST_{skin}) retrievals from infrared measurements from
67 satellites are taken in relatively transparent atmospheric “windows.” The atmospheric
68 transmissivity is very variable, mainly due to variations in the atmospheric water vapor
69 distribution, being ~ 0.98 across the $\lambda = 10\text{-}13\ \mu\text{m}$ window for cold, dry Arctic
70 atmospheres, but being reduced for moist, tropical marine atmospheres to ~ 0.35 at $\lambda = 11$

71 μm and ~ 0.23 at $\lambda = 12 \mu\text{m}$. These transmissivities are for vertical propagation through
72 the atmosphere, and are further reduced for propagation of the radiation along longer
73 slant-paths at non-zero zenith angles. The most common approaches to correct for the
74 radiative effects of the intervening atmospheres are based on measurements in spectral
75 bands at wavelengths close to $3.7 \mu\text{m}$, $11 \mu\text{m}$ and $12 \mu\text{m}$, where the atmospheric
76 transmissivity has a spectral dependence. Measurements in the shorter wavelength
77 spectral intervals in the $3.5\text{-}4.1\mu\text{m}$ range are contaminated during the daytime by
78 reflected sun glint at the surface or scattered solar radiation within the atmosphere; they
79 have generally been used during nighttime. The limited number of infrared window
80 channels in a single view has long been recognized as having insufficient information
81 content to permit the correction of the effects of aerosol variability as well as the full
82 range of air temperature and water vapor variability and air-sea temperature differences
83 (Merchant et al. 2006; Walton 2016). SST_{skin} retrievals depend on the algorithms being
84 suitable for the tasks; the errors and uncertainties of the derived variables being
85 confidently estimated, and the dependencies of estimated retrieval errors and
86 uncertainties on controlling parameters such as aerosol dust being well understood.

87 The attenuation of the upward-propagating surface infrared emission due to
88 aerosol dust has been studied extensively. For example, Nalli et al. (2012) and Nalli et al.
89 (2013) discussed the angular effects of aerosols in clear-sky radiance measurements, and
90 derived a simple physical conceptual model to quantify the infrared brightness
91 temperature sensitivity to aerosols and residual clouds that were not correctly identified
92 by cloud screening algorithms (Kilpatrick et al. 2019). The brightness temperatures
93 derived from measurements at satellite height are affected by the radiative path through

94 the dust layer, its shape and vertical concentration distribution, and temperature contrast
95 between the dust layer and sea surface. Building on earlier results which indicated poorer
96 accuracies of AVHRR-derived SST due to aerosols (Díaz et al. 2001), Arbelo et al.
97 (2003) reported a relationship between AVHRR-derived SST errors and aerosols by
98 comparisons with temperatures measured from satellites and drifting buoys in the area of
99 the Atlantic Ocean where Saharan dust outbreaks occur. The impact of aerosols on the
100 SST_{skin} retrievals from measurements of the Along-Track Scanning Radiometers (ATSR)
101 are much reduced because of the dual-view scan mechanism (Brown et al. 1997;
102 O'Carroll et al. 2012), whereas the SST_{skin} retrievals of the linear-scanning AVHRR are
103 very susceptible to the effects of desert aerosol dust. Vázquez-Cuervo et al. (2004) found
104 the differences between ATSR-2 and AVHRR SST retrievals varied regionally, being
105 most significant in the Sahara dust region. Luo et al. (2020a) found that SLSTR
106 (Merchant 2012) SST_{skin} retrievals could be affected by Sahara aerosol dusts. Aerosol
107 optical depth (AOD) is a measure of the aerosol concentration in the atmosphere derived
108 by integrating the aerosol attenuation coefficient along the propagation path. Bogdanoff
109 et al. (2015) demonstrated the sensitivity of AVHRR SST retrievals to the vertical
110 distribution of aerosol dust layers using a radiative-transfer model: the error was found to
111 be over 1 K for 0.25 AOD and concluded that the dust layer thermal infrared influence at
112 various heights should be considered when attempting to improve the accuracy of
113 infrared satellite SST retrievals.

114 Aerosol particles absorb, scatter and emit infrared radiation; thus, the satellite-
115 measured radiation at the top of the atmosphere should be corrected for these effects
116 before an unbiased SST_{skin} can be derived. Efforts to establish a scheme to minimize the

117 errors due to aerosols have been made for many years (Blackmore et al. 2012; Marullo et
118 al. 2010). Nalli and Stowe (2002) presented a daytime dust correction method for
119 AVHRR onboard NOAA satellites, in which the reflectance ratio between AVHRR
120 channel 1 ($\lambda = 0.58$ to $0.68 \mu\text{m}$) and channel 2 ($\lambda = 0.75$ to $1.1 \mu\text{m}$) was sensitive to the
121 AOD. The empirically derived aerosol correction method was shown to reduce notably
122 the SST differences with respect to buoy observations. Merchant et al. (2006) proposed
123 the Saharan Dust Index (SDI) as a result of analysis of radiative transfer model
124 simulations of the measurements of the Spinning Enhanced Visible and InfraRed Imager
125 (SEVIRI), SDI is used to correct the SST retrieval algorithms with an empirical
126 expression; the results showed an average of 0.2 K error was removed for SEVIRI SST
127 retrievals; and Le Borgne et al. (2013) used the same method for VIIRS onboard S-NPP,
128 the standard deviation was reduced by an amount in the range of 0.1 K to 0.15 K for
129 VIIRS. For the Along-Track Scanning Radiometers (ATSRs), Good et al. (2012) derived
130 the ATSR Saharan dust index (ASDI) with the principal component analysis of the
131 brightness temperature differences of selected channels; the second principal component
132 was related to AOD and can be used to effectively detect the mineral dust. More recently,
133 Luo et al. (2019) developed a night-time Dust-induced SST Difference Index (DSDI) for
134 MODIS onboard the AQUA satellite; the average SST differences were reduced by 0.16
135 K near Saharan dust regions, dependent on the MODIS data quality level.

136 Radiative transfer simulations of the SST_{skin} errors show they are related to the
137 dust layer temperature and altitude; the SST_{skin} errors are directly attributable to the
138 aerosol dust influence on the satellite brightness temperatures. Following Nalli et al.
139 (2012), the infrared brightness temperature change δT_{Ba} due to aerosol dust optical depth

140 $\tau_{\lambda a}$ for an idealized “super window” (an idealized super-transparent micro-window with
 141 negligible attenuation by gases) can be theoretically written as

$$142 \quad \delta T_{Ba}(\lambda, \theta, \tau_{\lambda a}, T_s, \bar{T}_a) \approx [1 - \exp(-\tau_{\lambda a} \sec \theta)] \frac{\left[\frac{\partial B_\lambda}{\partial T} \right]_{\bar{T}_{Sa}}}{\left[\frac{\partial B_\lambda}{\partial T} \right]_{\bar{T}_B}} \delta T_{Sa} \quad \text{Equation (1)}$$

143 where δT_{Ba} is the difference between the clear sky brightness temperature and the
 144 aerosol-contaminated brightness temperature, δT_{Sa} is the temperature difference between
 145 the surface and dust layers, \bar{T}_{Sa} is the average of the temperatures of the surface and the
 146 dust layer, θ is the satellite zenith angle, B_λ is the black body spectral radiance at
 147 wavelength λ . \bar{T}_B is the “observed” average brightness temperature of the surface and
 148 dust layer. The vertical distribution of aerosols has a significant impact on the
 149 atmospheric heating rate profile; aerosol dust changes the air temperature by absorbing
 150 and emitting infrared radiation. The vertical distribution of aerosols is related to the
 151 temperature of the aerosol layer, which then affects the infrared brightness temperatures.
 152 Also, the secant of the satellite zenith angle (θ) represents the increase in the optical path
 153 of the dust layer along an inclined propagation path, and consequences on the observed
 154 brightness temperature (Le Borgne et al. 2013).

155 Most of these studies addressed the effects of aerosol dust on the accuracy of the
 156 infrared satellite-derived SST_{skin} determined by comparisons with drifting buoy
 157 measurements, which have thermometers mounted typically 20 cm below the sea surface.
 158 However, the temperature variability between that depth and the surface contributes to
 159 the differences between the satellite-derived and buoy temperatures. The study reported
 160 here used remotely sensed SST_{skin} from the Marine-Atmosphere Emitted Radiance

161 Interferometers (M-AERI; Minnett et al. (2001)) mounted on research vessels to assess
162 MODIS SST_{skin} under Saharan aerosol dust outflows, thereby removing the uncertainties
163 introduced by temperature variability beneath the ocean-atmosphere interface.

164 This study focuses on the effects of aerosol dust on Terra MODIS-derived SST_{skin} ,
165 particularly the impact of the vertical distribution of the dust, and provides some
166 suggestions for improving the accuracy of the SST_{skin} retrievals. In addition to the M-
167 AERI SST_{skin} data, radiosonde air temperature and water vapor profiles collected from
168 research cruises onboard the NOAA Ship *Ronald H. Brown (RHB)* and R/V *Alliance*
169 were used. In Section 2, we introduce the MODIS TERRA SST_{skin} retrieval algorithms,
170 the M-AERI and radiosonde measurements, the Modern-Era Retrospective Analysis for
171 Research and Applications, Version 2 (MERRA-2; Gelaro et al. (2017)) dust profile data,
172 Radiative Transfer for TOVS (RTTOV; Saunders et al. (2018)) model, and give an
173 overview of the AERosols and Ocean Science Expeditions (AEROSE) ship-based field
174 campaigns. Section 3 describes the in-situ match-up results. Section 4 provides a detailed
175 quantitative analysis of the SST_{skin} differences through the use of radiative transfer
176 simulations, including the effects of the temperature and height of the dust layer. Section
177 5 concludes the paper with a summary of our approach and findings.

178 **2. Instruments and data**

179 **2.1 MODIS satellite data**

180 The TERRA MODIS SST_{skin} retrievals from 2007 to 2019 are used in this study.
181 Level 2 SST_{skin} data files were downloaded from <https://disc.gsfc.nasa.gov/>. Each L2
182 SST_{skin} pixel contains a Quality Level (QL) indicator, with 0 indicating best quality and 4
183 the worst quality. We use in this study QL = 0, QL = 1 and QL = 2 data, the “best”,

184 “acceptable”, and “suspect” quality data. QL = 0 and 1 data are preferred since they
 185 should be more accurate than those with QL = 2. As described in the MODIS SST_{skin}
 186 quality level flow chart (GSFC 2020), SST retrievals 3 K colder than a reference SST are
 187 assigned to QL = 2; however, the aerosol dust could introduce more than 3 K error in the
 188 retrieval, which is why QL = 2 data are included in this study. Also, there is a limit for
 189 situations where the impact of aerosols is so strong to produce situations similar to cloud
 190 cover.

191 The current MODIS SST_{skin} retrieval algorithm (GSFC 2020) is derived using a
 192 slightly modified nonlinear SST algorithm (NLSST; Walton et al. (1998)):

$$193 \quad SST_{skin} = a_{ij0} + a_{ij1}BT_{11\mu m} + a_{ij2}(BT_{11\mu m} - BT_{12\mu m}) \times T_{sfc} + a_{ij3}(\sec(\theta) -$$

$$194 \quad 1) \times (BT_{11\mu m} - BT_{12\mu m}) + a_{ij4} \times M + a_{ij5}(\theta) + a_{ij6}(\theta)^2 \quad \text{Equation (2)}$$

195 Where $BT_{11\mu m}$ and $BT_{12\mu m}$ are the top-of-atmosphere brightness temperatures derived
 196 from radiance measurements in the 11 and 12 μm bands. M is the mirror side. T_{sfc} is the
 197 “first guess” SST based on SST4 4 μm retrievals during nighttime and the Canadian
 198 Meteorological Center SST (Brasnett 2008) during daytime. T_{CMC} scales the brightness
 199 temperature difference correction due to water vapor column amount which is related to
 200 T_{sfc} (GSFC 2020; Walton et al. 1998). θ is satellite zenith angle. M is used to correct the
 201 potential differential degradation between the spectral reflectivity of the two mirror
 202 sides. a_{ij0} to a_{ij6} are the atmospheric correction coefficients derived with matched in-situ
 203 SST (Kilpatrick et al. 2015). Unlike the SLSTR on Sentinel-3a and -3b (Donlon et al.
 204 2012; Merchant 2012) which have coefficients of the atmospheric correction algorithm
 205 derived through radiative-transfer modelling (Embury and Merchant 2012; Embury et al.
 206 2012; Merchant 2012), the MODIS atmospheric correction coefficients are derived from

207 regressions between MODIS brightness temperatures and collocated, coincident in-situ
208 temperature measurements, and are set according to the month of year (i) and latitude
209 bands (j).

210 The MODIS SST_{skin} atmospheric correction algorithm has been frequently updated,
211 and the MODIS data have been reprocessed accordingly, so as to provide consistent high-
212 quality fields by using improved atmospheric correction algorithms and cloud masks. The
213 development of the MODIS NLSST algorithm is discussed by Brown and Minnett (1999),
214 Kilpatrick et al. (2001), and Kilpatrick et al. (2015).

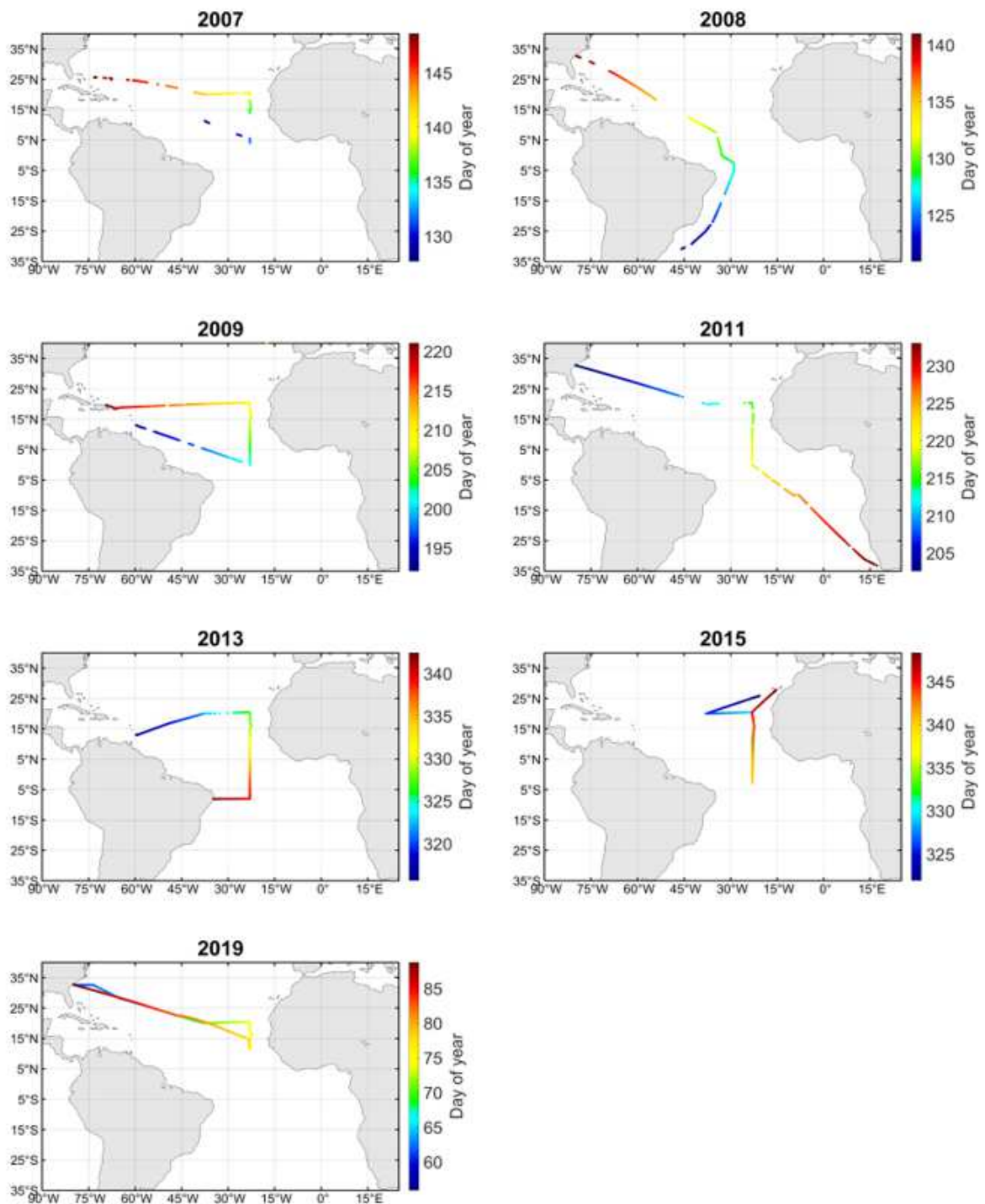
215 **2.2 AEROSE cruises**

216 All of the M-AERI and radiosonde data used here are from a series of AEROSE
217 cruises (Morris et al. 2006; Nalli et al. 2011) in the tropical and subtropical Atlantic
218 Ocean. Measurements taken during these cruises permit the quantification of the effects
219 of Sahara dust aerosol on satellite retrievals and reanalysis fields. SST_{skin} is derived from
220 M-AERI measurements. Radiosondes were launched from the ships every 4-8 hours
221 depending on satellite overpass times. By using a total of 650 radiosondes from the
222 AEROSE cruises, this study offers a valuable way to validate satellite SST_{skin} retrievals
223 through atmospheres containing mineral dust and dry air layers originating from Africa;
224 the dry layer effects on SST_{skin} retrievals from the measurements of MODIS on AQUA
225 have been discussed by Szczodrak et al. (2014).

226 Table 1 summarizes the time, coverage, and the number of radiosondes deployed
227 on the *RHB* and *Alliance*. Figure 1 shows the tracks of the ships; all of the plotted data
228 points have valid M-AERI measurements which enable the study of the effects of the
229 aerosol vertical distribution on the accuracies of the TERRA MODIS SST_{skin} products.

Table 1. Details of the AEROSE cruises used in this study.

CRUISES	NUMBER OF RADIOSONDES	START	END	DAYS OF DATA
2007 RHB	96	2007-05-07	2007-05-28	22
2008 RHB	74	2008-04-29	2008-05-19	21
2009 RHB	78	2009-07-11	2009-08-11	31
2011 RHB	102	2011-07-21	2011-08-20	31
2013 RHB	111	2013-11-11	2013-12-08	28
2015 Alliance	92	2015-11-17	2015-12-14	28
2019 RHB	97	2019-02-24	2019-03-29	34
Total	650	2007-05-07	2019-03-29	195
RHB: NOAA Ship <i>Ronald H. Brown</i> .				
Alliance: North Atlantic Treaty Organization (NATO) R/V Alliance.				

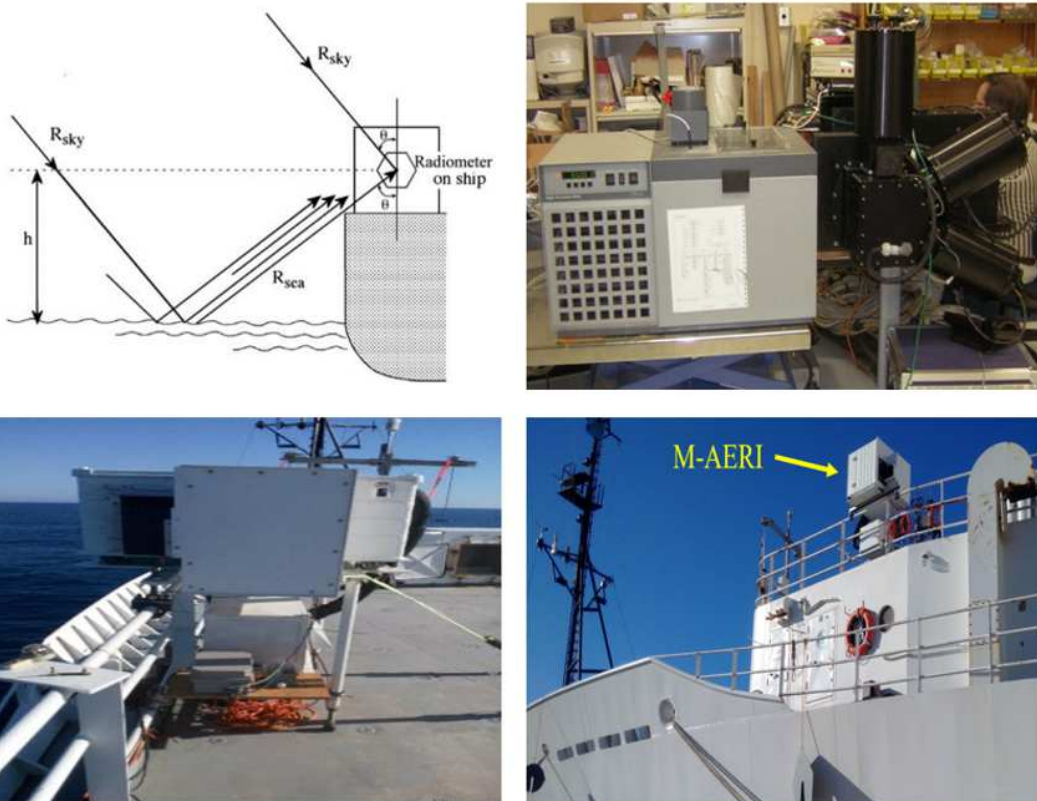


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233 *Figure 1. Cruise tracks of each AEROSE campaign. The colors indicate the day of year.*
 234 *Gaps indicate where M-AERI measurements were not made due to the instrument*
 235 *entering safe mode during rain or sea-spray events, or instrument repairs.*

236 **2.2.1 M-AERI**

237 M-AERIs are hyperspectral interferometric Fourier Transform Infrared (FTIR)
238 radiometers that measure the infrared emission spectra of the ocean surface and
239 atmosphere from which SST_{skin} can be derived (Minnett et al. 2001). These are directly
240 comparable to the MODIS SST_{skin} retrievals. M-AERIs are mounted a few meters above
241 the sea surface on the ships, as shown in Figure 2 (bottom).



242
243 *Figure 2. Top left: Viewing geometry of M-AERI. Top right: The M-AERI internal*
244 *calibration is checked in the laboratory before and after each deployment using an*
245 *external calibration procedure. Bottom: Installations of M-AERI on the NOAA ship*
246 *Ronald H Brown (RHB). The M-AERIs are inside hermetically sealed aluminum*
247 *enclosures with only the scan mirror and calibration black-bodied being exposed to the*
248 *open air, but protected. The smaller boxes beneath contain air-conditioning units that*
249 *limit temperature and humidity variations in the instrument enclosures.*

250 Figure 2 (top left) shows the viewing geometry of M-AERI; two internal
251 blackbodies provide a two-point calibration before and after each measurement of the
252 sea-surface and sky infrared emission spectra. The sky radiance reflected from the sea
253 surface is corrected using the sky emission measurements as described by Minnett et al.
254 (2001). The M-AERI SST_{skin} is derived from measurements at a wavelength of $7.7 \mu\text{m}$ to
255 reduce the sensitivity to atmospheric variability (Smith et al. 1996). Figure 2 (top right)
256 shows the M-AERI calibration being checked in our laboratory, which happens before
257 and after each deployment, by measuring the emission from a water-bath calibration
258 target of National Institute of Standards and Technology (NIST) design (Fowler 1995)
259 which has calibration traceability to standards at NIST (Rice et al. 2004) and at the UK
260 National Physical Laboratory (Theocharous et al. 2019). The M-AERI data are extremely
261 useful to provide measurements for validating and improving satellite-derived variables
262 (Luo et al. 2019; Szczodrak et al. 2014) and reanalysis products (Luo and Minnett 2020;
263 Luo et al. 2020b) under various situations.

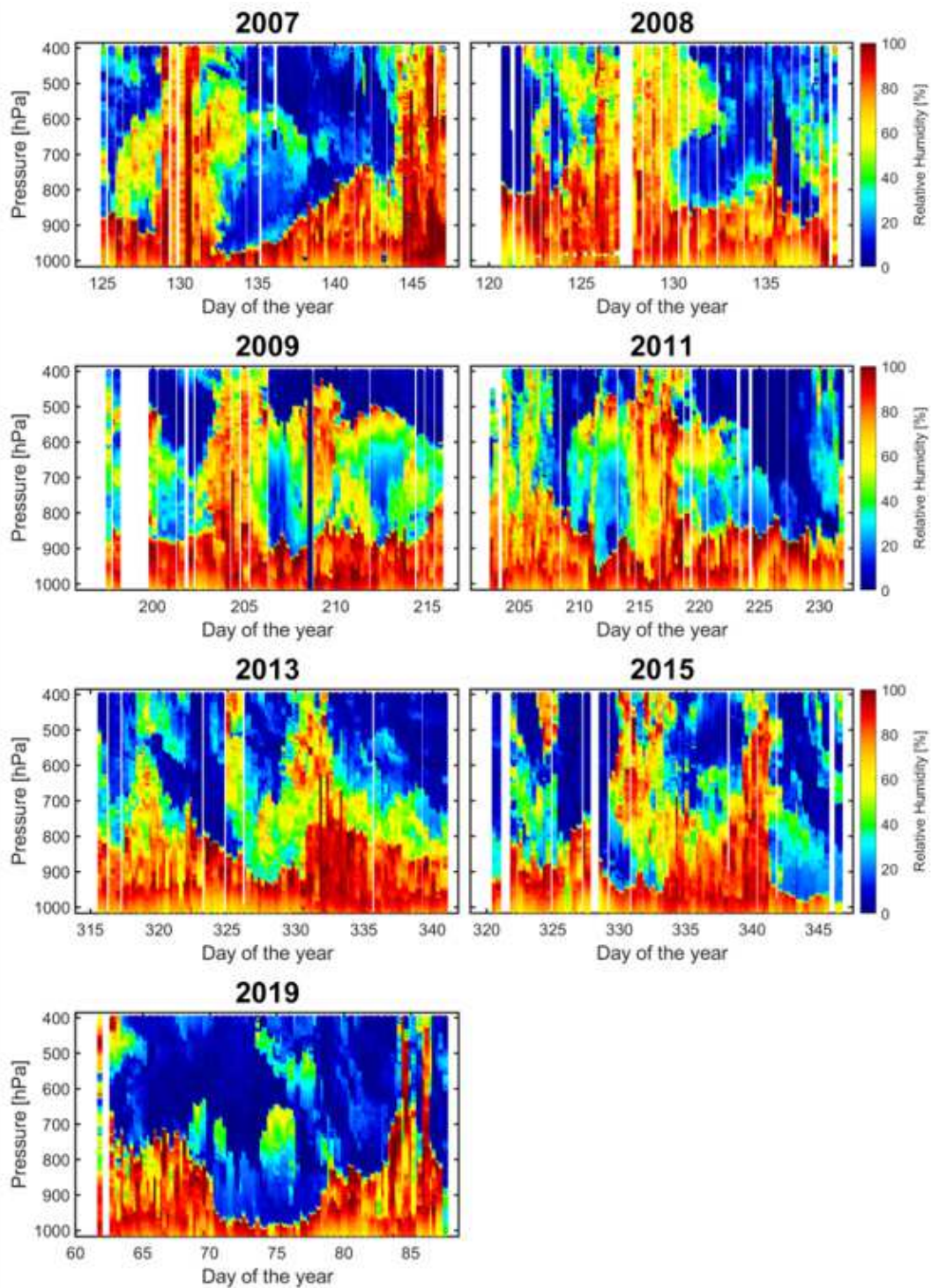
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265 **2.2.2 Radiosondes**

266 Vaisala RS92 radiosondes were launched during the AEROSE campaigns to
267 measure atmospheric values of temperature and humidity. Radiosondes take
268 measurements every second from the surface to typically 100 hPa, which results in a very
269 high vertical resolution (~ 0.1 hPa) depending on the speed of ascent. Radiosonde data
270 provide input for the radiative transfer model to simulate the MODIS measurements
271 under various aerosol dust loads, derived from the MERRA-2 fields, to assess the
272 degradation of the accuracies of the MODIS SST_{skin} retrievals. The radiosonde data

273 indicate the presence of anomalies in the atmospheric profiles, such as dry layers or the
274 near-surface warm dust layer. Atmospheric relative humidity and air temperature sections
275 from radiosondes along the cruise tracks (Figure 1) are presented in Figures 3 and 4. The
276 x-axes are the day of the year.

277



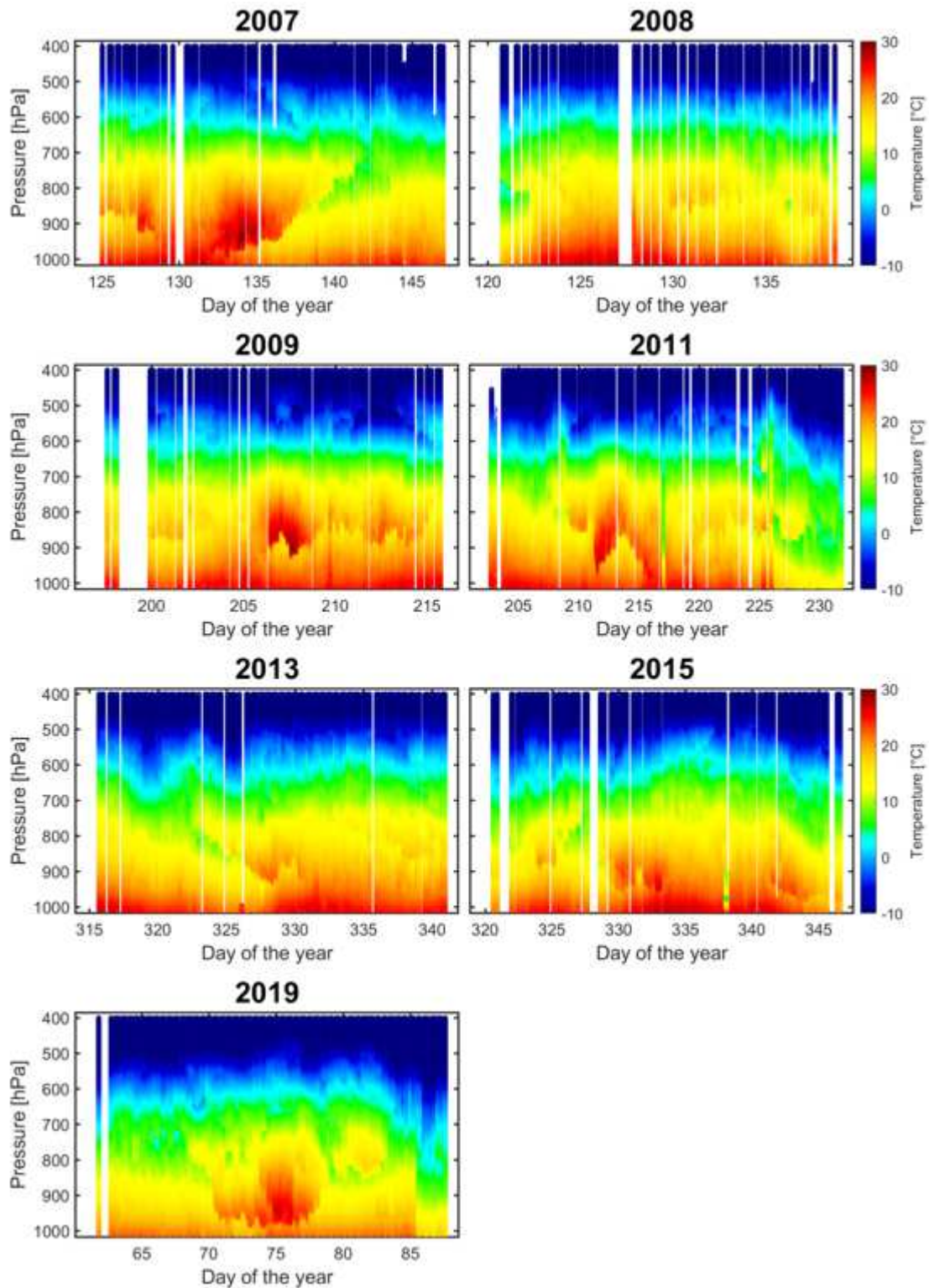
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Figure 3. Relative humidity measured by radiosondes launched from the ships. Colors

280

indicate the relative humidity. The dust dry layers are clearly visible on days 135-142 of

281 2007, 127-131 of 2008, 205-210 of 2009, 210-215 of 2011, 325-333 and 341-347 of 2015,
282 and 68-79 of 2019, usually from the surface to 700 hPa.



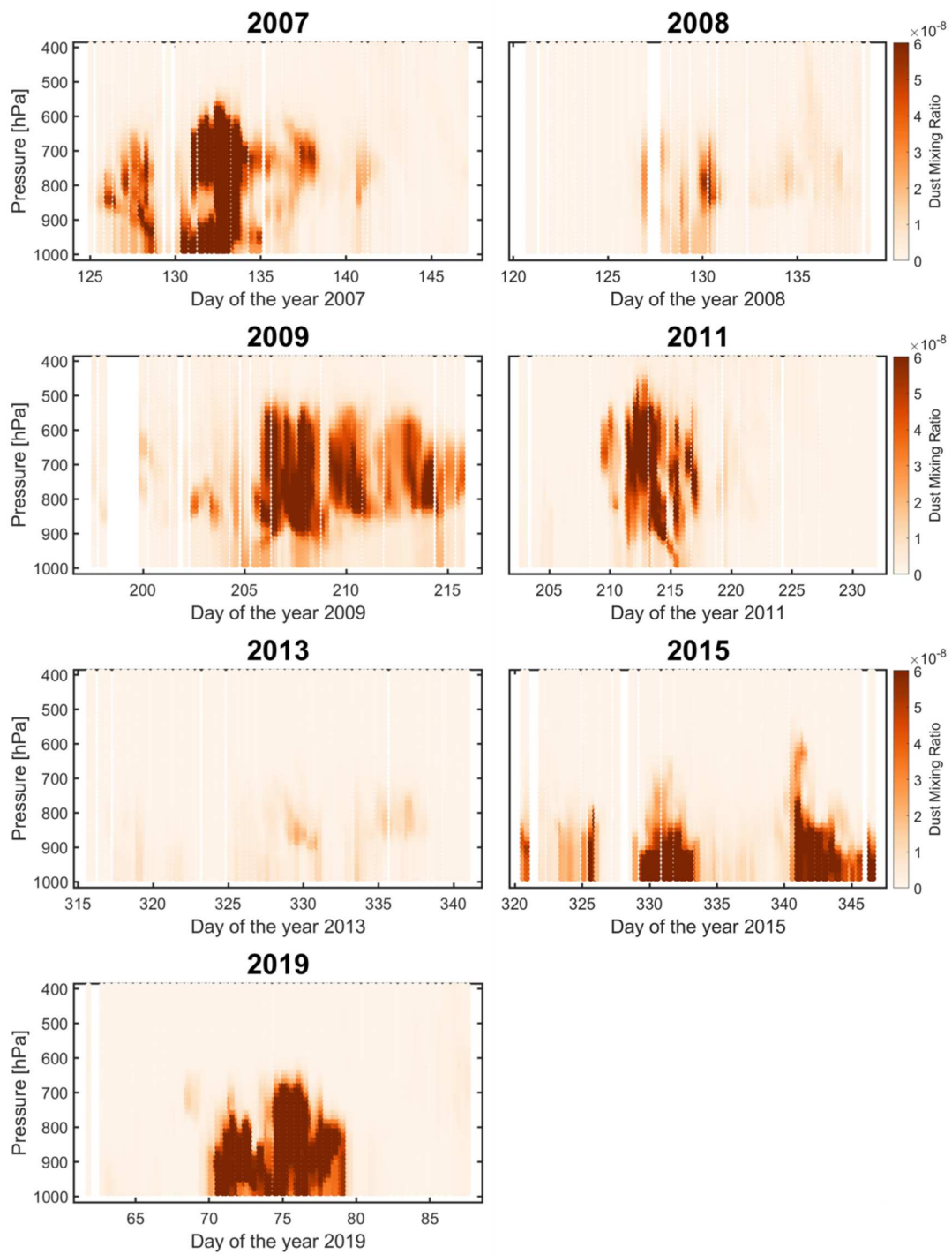
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 284 *Figure 4. As Figure 3, but for air temperature. The color indicates temperature*
 285 *according to the scale at right. The unit is °C.*

286

287 **2.3 MERRA-2**

288 The MERRA-2 reanalysis model output was generated in NASA's Global
289 Modeling and Assimilation Office Data Assimilation System (Bosilovich et al. 2015;
290 Gelaro et al. 2017) and is available through <http://disc.sci.gsfc.nasa.gov/mdisc/>. MERRA-
291 2 fields are calculated on a regular geographic grid at a spatial resolution of
292 approximately $0.625^\circ \times 0.5^\circ$ in longitude \times latitude. The MERRA-2 data contain
293 geolocated, derived geophysical variables, including aerosol dust mixing ratio used in
294 this study, at 72 standard pressure levels. MERRA-2 assimilates the dust profile from
295 various ground-based as well as space-based sources; details of the MERRA-2 dust
296 profile assimilation is described by Randles et al. (2017). MERRA-2 has five size bins for
297 dust aerosols spanning $0.1 \mu\text{m}$ to $10 \mu\text{m}$ radius, from which the subsets of bin 2 ($1 \mu\text{m}$ to
298 $1.5 \mu\text{m}$) and bin 3 (from $1.5 \mu\text{m}$ to $3 \mu\text{m}$) were used in this study, since they are more
299 widely spatially distributed (Haywood et al. 2005) and have a strong effect on IR
300 radiative transfer.

301 We use dust mixing ratio values from MERRA-2 to conclude the effects of the
302 vertical aerosol dust outbreaks on MODIS derived SST_{skin} . Figure 5 shows the
303 corresponding MERRA-2 value. The MERRA-2 dust values used in this study have a 3-
304 hour temporal resolution (Buchard et al. 2017; McCarty et al. 2016; Randles et al. 2017);
305 MERRA-2 aerosol values were linearly interpolated in time and bi-linearly interpolated
306 in space to the ship positions and times.



307
 308
 309

Figure 5. MERRA-2 dust mixing ratio sections of each AEROSE track, only the days with valid radiosonde data are plotted. Color indicates dust mixing ratio as shown on the

310 *right. White vertical lines indicate where radiosondes were not deployed due to inclement*
311 *weather or other reasons. The dust mixing ratio is kg/kg.*

312 **2.4 RTTOV**

313 RTTOV is a fast radiative transfer model developed by the UK Met Office and
314 Météo-France within the Numerical Weather Prediction Satellite Application Facility
315 (NWP-SAF) (Saunders et al. 2018). RTTOV simulates measurements of radiometers on
316 satellites, and is widely used by satellite remote sensing communities. Simulations of
317 brightness temperatures have many applications, such as improving MODIS SST_{skin}
318 retrievals under aerosol dust conditions (Luo et al. 2019), and developing cloud mask for
319 operational SST retrieval (Merchant et al. 2005), etc. Air temperature and relative
320 humidity at pressure levels through the atmosphere, SST_{skin} , and other inputs are needed
321 to perform brightness temperature calculations. Measurements from radiosondes and M-
322 AERIs, and the aerosol information from MERRA-2, described above, provide the
323 atmospheric and surface parameters for the brightness temperature calculation. RTTOV
324 version 12.3, used here, is available from <https://www.nwpsaf.eu/site-/software/rttov/>.

325

326 **3. SST_{skin} Assessment**

327 This study investigated the aerosol dust effects on the SST_{skin} retrievals from
328 MODIS against the well-calibrated M-AERI SST_{skin} values in the Atlantic Ocean. It is
329 necessary to note that this study only examines the TERRA MODIS SST_{skin} data with a
330 $QL < 3$ and pixels that have been confidently identified as being cloud contaminated are
331 not used.

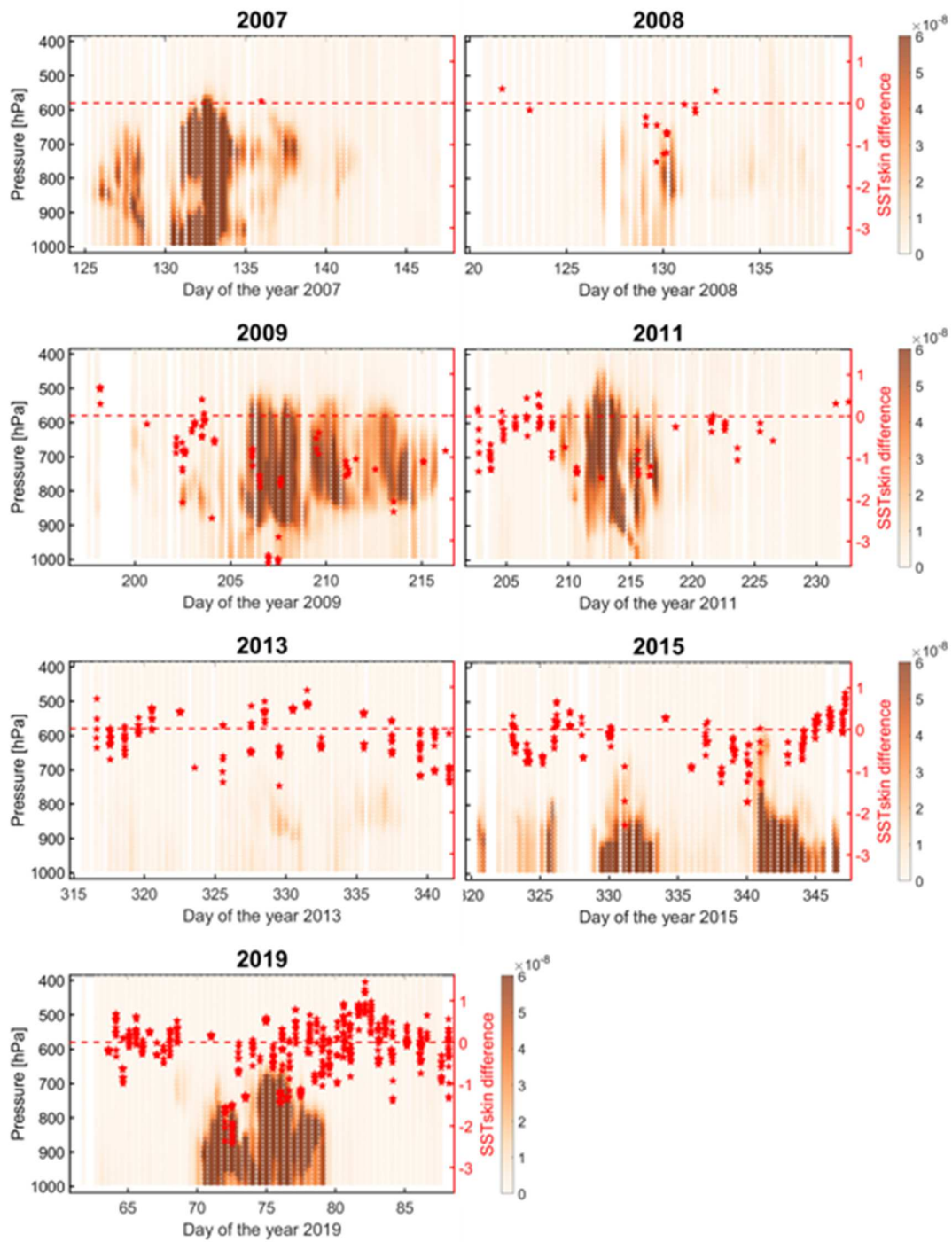
332 A Match-Up Data Base (MUDB) was generated to compare the MODIS SST_{skin}
333 fields with M-AERI SST_{skin} retrievals. ‘match-up’ stands for a data vector that consists of
334 MODIS derived SST_{skin} , M-AERI SST_{skin} , MERRA-2 dust concentrations, and other
335 relevant parameters. Match-ups are co-located between satellites and M-AERI data taken
336 within 30 minutes and 10 km of latitude and longitude (Donlon et al. 2014a; Kilpatrick et
337 al. 2015). Additional variables are included in each MUDB record, including the MODIS
338 infrared brightness temperatures and parameters of the satellite instrument viewing
339 geometry.

340 All of the AEROSE cruises included regions of Saharan dust outflow. The dust
341 can be lifted up to 500 hPa and transported over the North Atlantic Ocean as shown in
342 Figure 5. The dust mixing ratio distributions from MERRA-2 along the ship tracks
343 indicate large scale Saharan dust outflow on days 135-142 of 2007, 127-131 of 2008,
344 205-210 of 2009, 210-215 of 2011, 325-333 and 341-347 of 2015, and 68-79 of 2019.
345 Figures 3 and 4 show that the elevated dust layers are sometimes associated with dry air
346 layers; the dry layer effect on MODIS derived SST_{skin} has been discussed by Szczodrak et
347 al. (2014) who found that anomalous dry layers can introduce both positive and negative
348 errors in MODIS SST_{skin} retrievals dependent on the height of dry layers. However, there
349 were some days when the dry layers were not associated with dust layers, such as the
350 days 135-140 of 2008 and the days 220-232 of 2011; also there were some days the dust
351 was in moist layers such as the days 130-132 of 2007 and the days 214-216 of 2011. The
352 dust may absorb the shortwave radiation and warm the lower tropospheric temperature
353 (Choobari et al. 2014; Twomey 1972), also as shown in the radiosonde measured air
354 temperature (Figure 4). The air temperature and relative humidity anomalies associated

355 with aerosol dust layers were captured by the radiosonde data used in this research.
356 Therefore, the AEROSE cruises provide an opportunity to test the accuracies of the
357 MODIS SST_{skin} values under a variety of meteorological conditions.

358 This study is limited to conditions in which the cloud screening algorithms
359 indicate cloud-free skies as the match-up pairs have been subjected to the updated cloud
360 mask (Kilpatrick et al., 2019b). The SST_{skin} differences are defined as MODIS minus M-
361 AERI. To illustrate the aerosol dust effects, Figure 6 shows the SST_{skin} differences and
362 MERRA-2 dust mixing ratios (Figure 5), as a function of time along the ships' tracks,
363 according to the color bar at the right side.

364



365

366 *Figure 6. SST_{skin} difference from each of the ship tracks. Red stars indicate the difference*
 367 *with the right y-axis range. The operations of M-AERIs are suspended during rain thus*

368 causing some SST_{skin} data gaps along the track. Comparisons in and close to ports are
369 not used. The background color indicates the MERRA-2 dust mixing ratio.

370 Although the AEROSE 2008 cruise has relatively few match-up points, the
371 available pairs around days 127-131 show colder MODIS SST_{skin} temperatures when dust
372 is present (Figure 6), and although the dust concentration is quite small, it occurs at high-
373 altitude and its relatively cold temperature ($12^{\circ}\text{C} - 14^{\circ}\text{C}$ for dust layers and $27^{\circ}\text{C} - 30^{\circ}\text{C}$
374 for SST_{skin}) leads to a comparable MODIS SST_{skin} retrieval error to situations where
375 denser dust layers occur lower in the atmosphere, such as in 2015 and 2019. There are
376 strong Saharan dust outbreaks along the AEROSE 2009 tracks across the Atlantic Ocean
377 (Figure 1). The SST_{skin} difference is positive at the beginning of the 2009 cruise in the
378 absence of dense dust, but being in the range of minus 1 K to 0 K for days 202-204 when
379 the dust concentration was moderate. On the days when the *Ronald H. Brown* entered
380 significant, large-scale Saharan dust outflow events, the negative SST_{skin} differences were
381 more pronounced: the averaged SST_{skin} difference being as large as -3 K between days
382 205-210. AEROSE 2011 also encountered a strong dust outbreak, with the averaged
383 SST_{skin} difference being $\sim 1\text{K}$ for days 210-216. The dust-layer temperature was high
384 ($22^{\circ}\text{C} - 28^{\circ}\text{C}$ for dust layers and $23^{\circ}\text{C} - 26^{\circ}\text{C}$ for SST_{skin}) during days 211-214 of 2011,
385 as shown in Figure 4, indicating a dry, warm dust layer which resulted in negative
386 MODIS SST_{skin} retrieval errors, but which are not as large as during AEROSE 2009. A
387 strong dust outbreak was not encountered during AEROSE 2013. Depending on other
388 factors, such as the characteristics of the dry layer, the SST_{skin} difference may be positive
389 or negative (Szczo drak et al. 2014). The 2015 AEROSE cruise was onboard the R/V
390 *Alliance*, and began on November 15 in Las Palmas, Gran Canaria, and ended on

391 December 14 in the same port, as shown in Figure 1. The Saharan dust outbreaks were
392 encountered many times during AEROSE 2015 (Figure 6), thus providing several sets of
393 measurements of the effects of dust outflow over the Atlantic Ocean. When the R/V
394 *Alliance* first entered a significant and large-scale Saharan dust outflow on days 323-326
395 of 2015, the dust layer extended in the vertical to ~850 hPa and the corresponding SST_{skin}
396 differences were in the range of ± 1 K. For the second Saharan dust encounter, on days
397 328-333, the SST_{skin} differences are negative, up to -2.5 K, with a dust layer with an
398 extensive vertical extent and high concentration. It is interesting to note that at the third
399 dust encounter from days 339-347, the SST_{skin} difference gradually changed from
400 negative to positive, possibly due to the dust layer altitude, humidity and temperature:
401 there were dry and warm anomalies at 850-1000 hPa, the positive SST_{skin} differences
402 during day 346 appear to have been caused by an anomalous warm temperature of the
403 dust layer near the port of Las Palmas, Gran Canaria. AEROSE 2019 began and ended in
404 Charleston, South Carolina. Most of the days during this cruise were under clear-sky
405 conditions; therefore, there are more match-up pairs between MODIS and M-AERI than
406 in other years. The MERRA-2 fields and radiosonde values clearly indicate the presence
407 of the warm and dry dust layer in days 70-77 (Figures 3 and 4). The results show a
408 pronounced SST_{skin} difference, sometimes more than -3 K, linked to the dust layer. The
409 overall SST_{skin} difference is negative, however, when the upper-tropospheric dust layer is
410 extremely warm and humid, as on day 75, the SST_{skin} difference is positive, ~0.8 K.

411 Equation (1) describes the theoretical sensitivity of top-of-atmosphere brightness
412 temperatures to an aerosol dust layer. The dust cooling effect can cause the temperature
413 difference between the surface and dust layers δT_{sa} to become negative, thus the

414 corresponding infrared brightness temperature, such as $BT_{11\mu m}$ and $BT_{12\mu m}$ in Equation
 415 (2), will decrease.

416 Combining Equation (1) and Equation (2), for the satellite zenith angle at nadir,
 417 and ignoring the small mirror-side term, the Terra MODIS SST_{skin} difference due to the
 418 $BT_{11\mu m}$ and $BT_{12\mu m}$ changes can be expressed as

419

$$\Delta SST_{skin} \approx b_{ij0} + [1 - \exp(-\tau_{\lambda a})] \times \delta T_{sa} \times \left\{ b_{ij1} \frac{\left(\frac{\partial B_{\lambda 11\mu m}}{\partial T}\right)_{\bar{T}_{Sa}}}{\left(\frac{\partial B_{\lambda 11\mu m}}{\partial T}\right)_{\bar{T}_B}} + b_{ij2} \times$$

$$T_{sfc} \left[\frac{\left(\frac{\partial B_{\lambda 11\mu m}}{\partial T}\right)_{\bar{T}_{Sa}}}{\left(\frac{\partial B_{\lambda 11\mu m}}{\partial T}\right)_{\bar{T}_B}} - \frac{\left(\frac{\partial B_{\lambda 12\mu m}}{\partial T}\right)_{\bar{T}_{Sa}}}{\left(\frac{\partial B_{\lambda 12\mu m}}{\partial T}\right)_{\bar{T}_B}} \right] \right\}$$

420

421

Equation (3)

422 b_{ij0} to b_{ij2} are the similar atmospheric correction coefficients as a_{ij0} to a_{ij6} in Equation
 423 (2). As shown in Equation (3), the SST_{skin} retrieval difference (ΔSST_{skin}) depends on the
 424 aerosol dust optical depth τ_{va} and the temperature difference between the surface and
 425 dust layers δT_{sa} , the results presented here are consistent with this simple expression.

426 Thus, expecting the SST_{skin} bias should be increased with the dust layer
 427 concentration and temperature difference with respect to the SST_{skin} , we define the
 428 following SST_{skin} bias factor (ΔSST_{aer_dT}) as

429

$$\Delta SST_{aer_dT} = \sum_{p=surface}^{p=400hPa} \sum_{i=3}^{i=1} (SST_{skin} - T_{air}) \times x_i \times \beta_{ext,i}$$

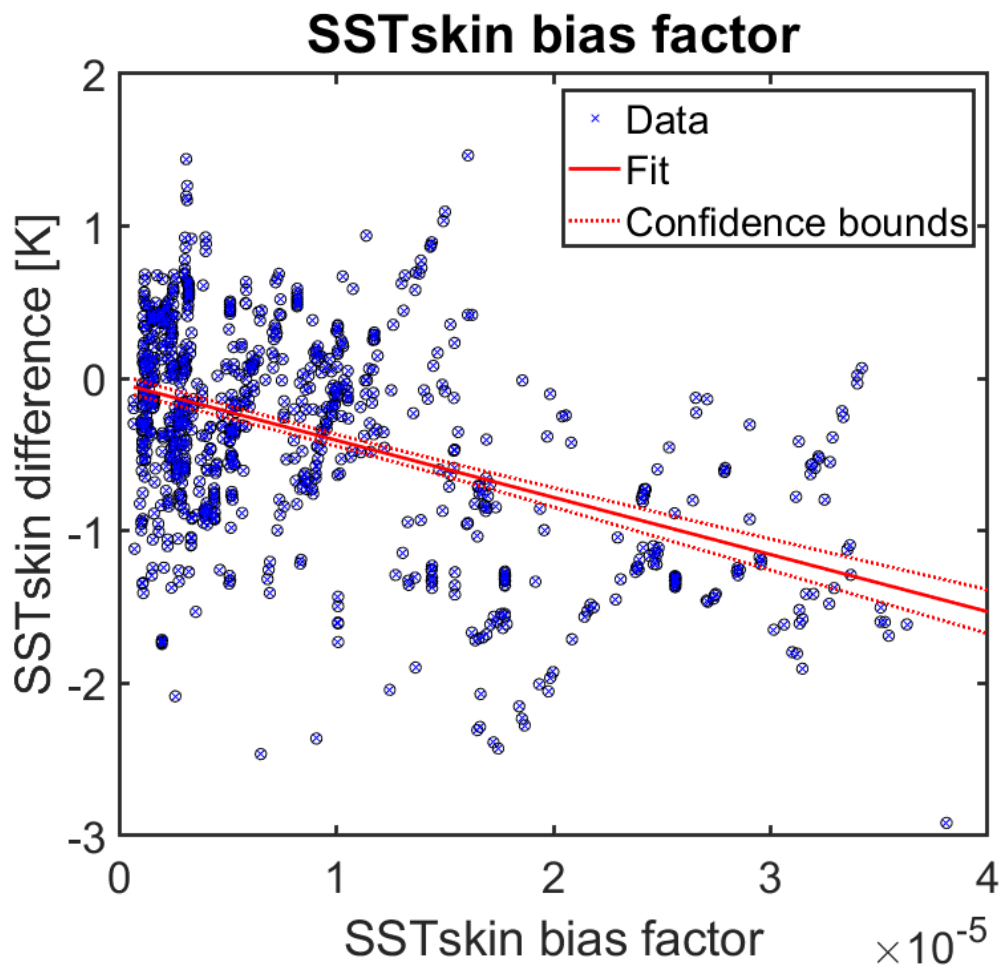
430

Equation (4)

431 Where x_i is each layer's MERRA-2 dust mixing ratio of bins 1, 2 and 3 with the
432 effective dust radii of 0.64, 1.34 and 2.32 μm , respectively, $\beta_{ext,i}$ is the sum of scattering
433 and absorption coefficients, as mass extinction coefficient of each dust bin, their values
434 are taken from supplementary tables of Randles et al. (2017). T_{air} is the air temperature
435 of the corresponding layer, SST_{skin} is the M-AERI measured skin temperature. The
436 ΔSST_{aer_dT} is integrated from the sea surface up to 400 hPa. Figure 7 shows the
437 relationship between ΔSST_{aer_dT} and the MODIS SST_{skin} retrieval bias. Only the match-up
438 pairs with MERRA-2 total AOD > 0.05 are included in Figure 7. There is an overall
439 negative correlation between them, when the $\Delta SST_{aer_dT} > 1.5 \times 10^{-5}$, the averaged
440 difference is > 1 K.

441

442



443

444 *Figure 7. The relationship between MODIS SST_{skin} retrieval bias and ΔSST_{aer_dT} .*

445 *The red line is the fitted linear regression line.*

446 As indicated by Brown and Minnett (1999), Merchant et al. (2006), Good et al.
 447 (2012), and Luo et al. (2019), the aerosol dust causes the split-window difference of
 448 $(BT_{11\mu m} - BT_{12\mu m})$ to decrease due to the spectral character of dust absorption in the
 449 long wavelength infrared window, thereby confounding the correction of the clear-sky
 450 atmospheric effect, due primarily to water vapor, in the SST_{skin} retrieval. Overall, the dust
 451 particles in the higher atmosphere introduce more negative errors into the retrieved
 452 SST_{skin} .

453 By using the AEROSE MUDB, this study revealed the impacts of the dust layer
454 vertical distribution on the MODIS-derived SST_{skin} . The comparison shows that the
455 infrared satellite-derived SST_{skin} negative differences are mainly localized in the Saharan
456 dust outflow region. The SST_{skin} retrieval error is related to the concentrations, altitudes,
457 and temperatures of dust layers.

458 **4. RTTOV Simulation Assessment and Discussion**

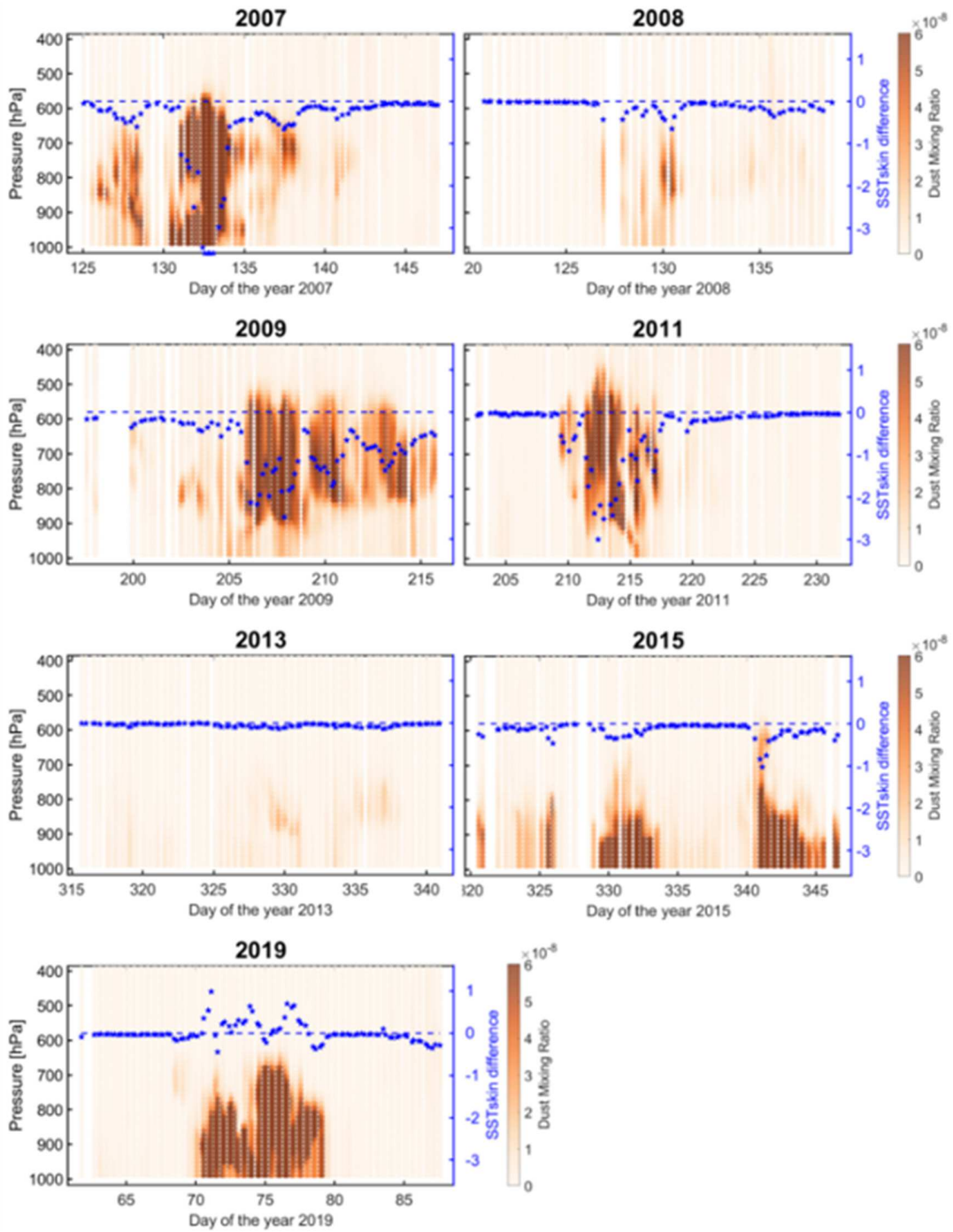
459 Inaccuracies in the TERRA MODIS retrieved SST_{skin} can be investigated by using
460 atmospheric radiative-transfer modeling. Brightness temperature simulations for TERRA
461 MODIS infrared channels 31 ($\lambda = 11 \mu\text{m}$) and 32 ($\lambda = 12 \mu\text{m}$) have been performed with
462 the RTTOV model, and the brightness temperatures are used to derive SST_{skin} according
463 to Equation 2. The internal RTTOV climatological type was held constant as “7:
464 Maritime polluted” to let the dust aerosol load over the ocean throughout the simulations.
465 The aerosol particle type was set as “Mineral Transported” from the Optical Properties of
466 Aerosols and Clouds index (OPAC; Hess et al. (1998))”. The RTTOV model was run
467 with radiosonde measured air temperature and humidity profiles and MERRA-2 dust
468 concentrations in Section 4.1, and with fixed atmospheric temperature and humidity but
469 with variable dust profiles in Section 4.2. In section 4.1, the MERRA-2 dust mixing ratio
470 was directly loaded into RTTOV for each pressure layer with the aerosol concentration
471 unit set as “kg/kg”. In section 4.2, simulations were conducted with varying dust
472 concentrations set at different vertical layers in the atmosphere. The solar and satellite
473 zenith angles are set to 0 in all the simulations to avoid the complications of slant path
474 attenuation as discussed by Nalli et al. (2012). The aerosol dust-induced SST_{skin} error
475 described in this section is defined as the dust aerosol-contaminated SST_{skin} retrieval

476 minus the “without dust” derived SST_{skin} , with a negative value indicating an error to
477 colder SST_{skin} retrievals due to the dust aerosol.

478 **4.1 Radiative Transfer Simulations**

479 Since the occurrence of the dust layer is often accompanied by clouds, such
480 SST_{skin} retrievals have been flagged as poor quality, for example, there are few match-up
481 pairs from the AEROSE 2007 cruise. However, we can use RTTOV to simulate the dust
482 effect on TERRA MODIS-derived SST_{skin} .

483



484

485 *Figure 8. SST_{skin} differences from RTTOV simulations along the cruise tracks. The blue*
 486 *stars indicate the simulated SST_{skin} error caused by the aerosol according to the y-axis*
 487 *scale at right. The background color indicates the MERRA-2 dust mixing ratio.*

488 Input for the aerosol-free RTTOV simulations are SST_{skin} from M-AERI, and air
489 temperature and humidity from radiosondes. We ran the RTTOV without dust aerosol to
490 simulate the TERRA MODIS clear-sky brightness temperature measurements, then
491 deriving the SST_{skin} using the standard MODIS NLSST atmospheric correction algorithm
492 (Equation 2). Dust mixing ratios from MERRA-2 are used to give the locations and
493 concentrations of the aerosol dust. The derivation of SST_{skin} was repeated with
494 simulations including the MERRA-2 dust values. The difference between the retrievals
495 reveals the SST_{skin} retrieval error under dust aerosol influence. Figure 8 shows the
496 RTTOV simulated results along each AEROSE cruise in this region; the blue stars are the
497 simulated SST_{skin} error associated with the right y-axis. The left y-axis indicates the
498 RTTOV pressure layer.

499 The results from AEROSE 2007 to 2011 show that the negative SST_{skin} difference
500 can be marked when the ship entered significant, large-scale Saharan dust outflow
501 regions. Moreover, the uncertainties are related to the dust layer thickness and altitude.
502 The intense dust outbreaks during days 132-133 of 2007, days 206-209 of 2009, and days
503 212-213 of 2011 can introduce simulated differences of -3 K to -4 K. AEROSE 2013 did
504 not encounter significant dust outbreaks; the low concentration dust layers during days
505 326-332 still introduced some SST_{skin} error, but within 0.05 K. The AEROSE 2015 passed
506 through a few Saharan dust outbreak regions, which can be seen in the background
507 MERRA-2 dust mixing ratio values. For days 340-342 of 2015, the thick dust layer,
508 extending from the surface to ~600 hPa introduced up to -1 K negative SST_{skin} retrieval
509 errors. The -1 K error is smaller than for 2007, 2009, and 2011, because the dust layer
510 was below 850 hPa for these days in 2015, so the dust layers were not lifted to higher

511 altitudes as in 2007, 2009 and 2011. The SST_{skin} difference is related to the dust layer
512 temperature; for a layer in the upper troposphere, it was found that both warming and
513 cooling effects can be introduced by dust. On the other hand, when the dust layer appears
514 in the lower troposphere, the warming effects dominate. The Saharan dust radiative
515 heating rates to the air temperature vary with the situation (Carlson and Benjamin 1980);
516 the maximum dust temperatures are usually near the maximum dust concentration level
517 and near the surface. The negative errors from days 343 to 347 of 2015 were thus
518 weakened because of the warm temperature of the dust layer. The AEROSE 2019 results
519 illustrate the warm dust layer effects on the simulated SST_{skin} : some of the simulated
520 errors are positive, up to 1K, for days 71-77. The results from in-situ validation (Section
521 3) and RTTOV simulations (Section 4.1) were reasonably consistent with each other,
522 indicating it is necessary to know the dust loading altitude and temperature to assess their
523 effects on satellite-derived SST_{skin} .

524 **4.2 McClatchey Standard Profile simulation**

525 Although the in-situ match-up measurements and RTTOV simulations
526 demonstrate a clear trend of an increasing error with denser and higher dust layers, the
527 SST_{skin} retrieval sensitivity to varying vertical distributions can be better determined by
528 simulations with a fixed atmospheric profile. Determining the sensitivity is the subject of
529 this section. The RTTOV model was run with fixed atmospheric conditions taken from
530 the McClatchey Standard Tropical Profile (McClatchey 1972), together with various dust
531 concentrations and vertical distributions. The fixed standard atmospheric profile makes it
532 possible to assess the impacts of the dust layer heights and dust layer temperature as all
533 other variables are held constant. Saharan dust outbreaks can be found at any height from

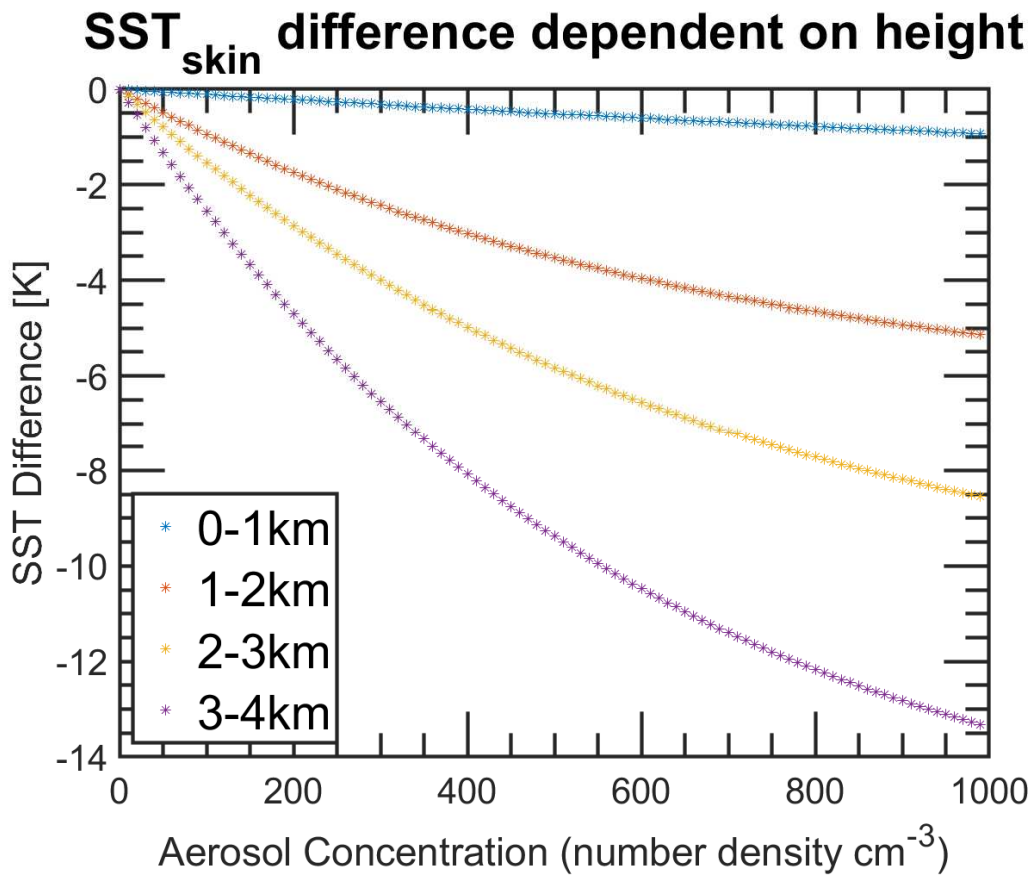
534 the surface up to 6 km, often depending on their transport ranges, sources and other
 535 environmental variables such as wind, air temperature, etc. (Karyampudi et al. 1999).
 536 Dust is inserted at four different altitudes in this study, corresponding to the defined
 537 RTTOV pressure levels shown in Table 2. The dust concentration is varied from 0 to
 538 1000 particles per cm⁻³, in increments of 10.

539 Table 2. Dust layer altitude range, corresponding RTTOV pressure layers
 540 and the mean air temperature of this layer.

Altitude	Pressure	Mean air temperature
0 km – 1 km	922 hPa, 957 hPa, 985 hPa, 1005 hPa	297K
1 km – 2 km	795 hPa, 839 hPa, 882 hPa	291K
2 km – 3 km	702 hPa, 749 hPa	286K
3 km – 4 km	610 hPa, 656 hPa	280.5K

541

542



543

544 *Figure 9. RTTOV simulation results showing the impact on the SST_{skin} retrieval of the*
 545 *altitude of the aerosol layer. Different colors indicate different altitudes of the dust layer.*
 546 *As the aerosol height is increased, the SST difference becomes more negative, except for*
 547 *very small concentrations.*

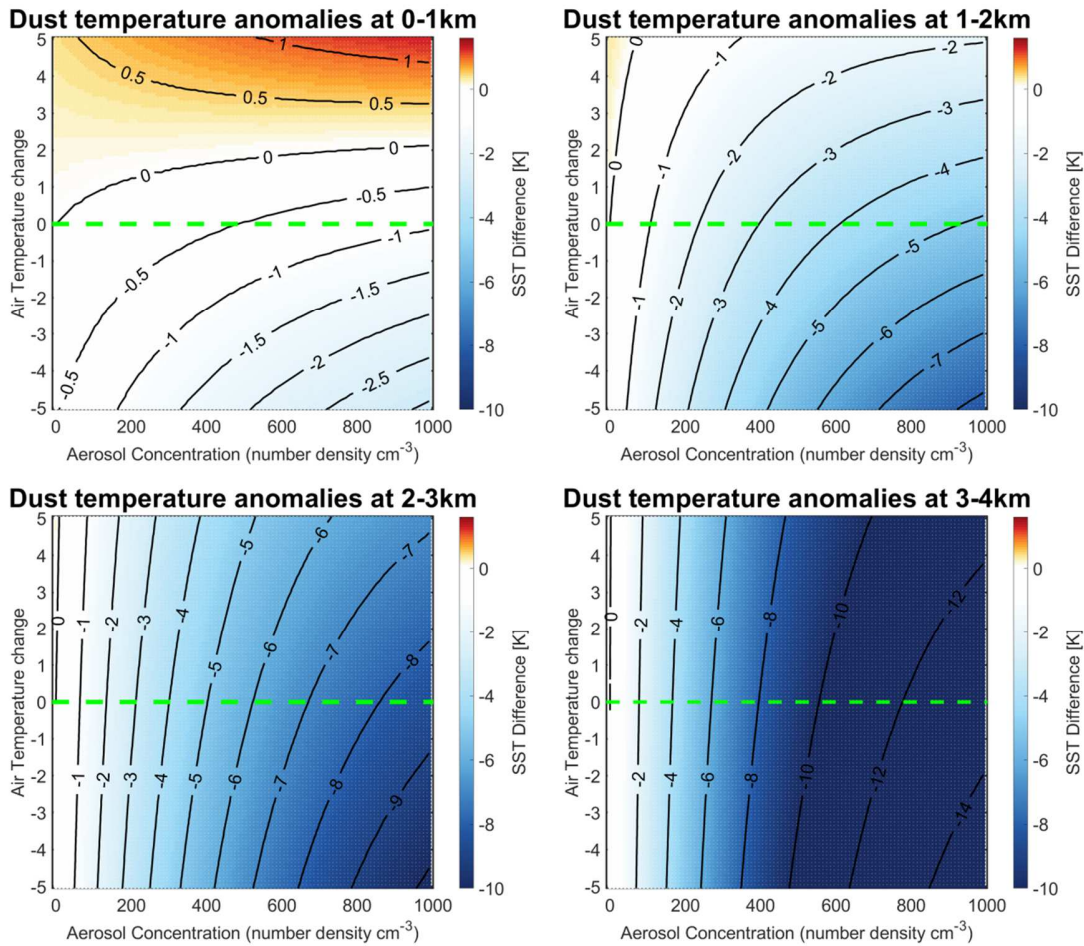
548 The SST_{skin} error introduced by dust aerosol is shown in Figure 9, with different
 549 colors indicating different altitude ranges into which the dust was inserted. All of the
 550 simulations show a cooling effect due to dust; as expected, the cooling varies over a
 551 range of aerosol concentrations and dust heights. As shown in Figure 9, dust present at
 552 lower altitudes introduces a smaller SST_{skin} error as the temperature contrast with the sea

553 surface is smallest. The only two variables in Figure 9 are difference in the simulated
554 SST_{skin} retrievals with and without dust aerosols, and dust aerosol concentrations.

555 To further investigate the physical mechanism of the aerosol effect on satellite-
556 derived SST_{skin} , this study explores the aerosol warming and cooling. Adebisi et al. (2015)
557 highlight the differences in the vertical temperature structure associated with different
558 AODs. The temperature of the boundary layer top is up to 2 K colder when aerosols are
559 present. The composite profile from polluted days ($AOD > 0.2$) reveals a previously
560 documented warmer temperature anomaly at a lower atmospheric layer around 1000 hPa,
561 capped by a colder anomaly at 600 hPa. Weaver et al. (2002) calculated the radiative
562 forcing of Saharan aerosol dust, finding an increase of TOA longwave radiation with
563 aerosol loading and observing that the aerosol dust absorbs infrared radiation and emits at
564 a lower temperature. Hansell et al. (2010) and Wong et al. (2009) also identified the same
565 vertical radiative effect of the Saharan dust layer: strong positive heating rates occur in
566 the lowest layers and the heating rates are negative in the upper troposphere.

567 As discussed above, the Saharan aerosol dust can introduce air temperature
568 anomalies according to their sources, altitude, or spatial distributions. The RTTOV model
569 simulations included modifications to atmospheric temperatures covering a range of
570 values that might result from the effects of the dust layers to determine their effects on
571 satellite-retrieved SST_{skin} . Figure 10 shows the results after adding positive or negative
572 temperature anomalies at different heights, indicated by the y-axis, with 0.1 K increments.
573 The input SST_{skin} was set to 298 K. This simulation study has used step functions of
574 adding the temperature anomalies to the aerosol layer. Evidence of dry layers in data
575 from radiosonde profile generality show a very sharp temperature and humidity changes

576 at both the lower and upper boundaries. To avoid statically unstable atmospheric
 577 situations, the temperature anomalies are limited as -5K to 5K.



578

579 *Figure 10. The effects on the SST_{skin} retrievals of the presence of air temperature*
 580 *anomalies of different magnitudes at various heights. The color indicates the SST_{skin}*
 581 *difference resulting from temperature changes in the aerosol layers. The x-axis is the*
 582 *aerosol concentrations at different heights as shown in the title. The y-axis is the aerosol*
 583 *layer temperature anomalies. The lines at $y = zero$ emphasize the change in sign of the*
 584 *air temperature anomalies. The results show that the SST_{skin} difference is related to the*
 585 *dust layer temperature change, dust concentrations and altitude.*

586 The parts above the green lines in Figure 10 illustrate the aerosol loading
587 conditions with warmer temperature anomalies in lower atmospheric layers. The thick
588 and warm dust layer load in the height range of 0-1 km can introduce differences in
589 derived SST_{skin} of up to 1.5 K; and the warm dust at heights of 1-2 km can also deliver
590 positive SST_{skin} retrieval differences. These results are comparable to those found in
591 Section 3 with in-situ measurements and MERRA-2 dust concentrations, such as towards
592 the end of AEROSE 2015 cruise under the Saharan dust, the dense and warm dust layer
593 near Las Palmas introduced a positive SST_{skin} error. The parts below the green lines in
594 Figure 10 show that the high-altitude dust over the tropical ocean contributes
595 considerably to the strong negative errors in those simulations.

596 As expected, introducing the cold temperature anomalies to the dust layer the
597 overall aerosol dust cooling effects are stronger in each simulation for the dust at various
598 altitudes. The bottom panels with dust present at 2-3 km and 3-4 km show a sharp
599 increase of negative errors in the simulations. The SST_{skin} difference is related to the dust
600 layer temperature; however, the aerosol concentration dominates the error. The aerosol
601 dust introduced SST_{skin} errors reach about -14 K when the thick aerosol layer occurs at 3-
602 4 km height, due to the relatively large temperature difference between the aerosol dust
603 layer and the sea surface. The magnitudes of this negative SST_{skin} error are in broad
604 agreement with those found in Bogdanoff et al. (2015) who investigated dust effects on
605 AVHRR SST_{skin} retrievals.

606 To summarize the results of the RTTOV simulations to investigate the impact of
607 aerosol dust on the SST_{skin} , the vertical distributions of aerosols influence the errors of
608 infrared-derived SST_{skin} . The errors are greater for higher dust layers, because higher dust

609 layers have a greater temperature difference to the sea surface. The magnitudes of the
610 negative SST_{skin} errors can be as large as -14 K in the case of dense and high dust layers,
611 occurring at 3-4 km height. On the other hand, a warm dust layer at lower altitudes can
612 introduce a positive SST_{skin} retrieval error.

613 The results indicate that improvements in atmospheric correction algorithms to
614 compensate for inaccuracies introduced by dust aerosol could be expected if efforts are
615 made to take dust layer concentrations, altitudes and temperatures into account. This
616 could be done by selecting coefficients in an NLSST-type algorithm that depend on prior
617 information on aerosol conditions, or using such aerosol information in an optimal
618 estimation approach (Merchant et al. 2008). Reliance on external aerosol information can
619 be avoided by including additional aerosol-sensitive channels in the atmospheric
620 correction algorithms (Luo et al. 2019; Merchant et al. 2006).

621

622 **5. Summary**

623 Instruments on the TERRA satellite provide a long-term, consistent and high-
624 quality set of data records of the Earth system. SST_{skin} , as one of the mature products
625 retrieved from MODIS onboard TERRA, has been developed and improved continually
626 for many research and operational applications such as climate change studies and
627 weather prediction. Although the MODIS onboard TERRA provides accurate estimates
628 of the SST_{skin} fields, the residual uncertainty characteristics due to such atmospheric
629 factors as aerosol dust cannot be ignored. This study aimed to improve the understanding
630 of the effect of the vertical aerosol dust distribution on infrared satellite-derived SST_{skin}

631 by using match-up methods as well as radiative transfer simulations. High-accuracy
632 shipboard derived SST_{skin} , using M-AERI, have been used to assess the aerosol dust
633 effects. Radiosonde and M-AERI data collected within Saharan dust outflow regions
634 during AEROSE cruises provide independent marine and atmospheric inputs for radiative
635 transfer simulations. The key findings are summarized below.

636 The results from in-situ match-ups and radiative transfer simulations are
637 comparable. Overall, the aerosol dust makes infrared SST_{skin} retrievals more negative; this
638 is in agreement with the results of correction for MODIS (Luo et al. 2019) , and
639 corrections for various sensors reported by other investigators (Blackmore et al. 2012;
640 Bogdanoff et al. 2015; Good et al. 2012; Le Borgne et al. 2013; Merchant et al. 2006;
641 Nalli et al. 2013). SST has been declared to be an Essential Climate Variable by the
642 Global Observing System for Climate (GCOS; Bojinski et al. (2014)) with required
643 measurement uncertainty of 0.1 K over 100 km scales (GCOS 2019). The SST_{skin} retrieval
644 errors introduced by aerosol dust layers are significant in comparison to the requirements
645 for the generation of SST Climate Data Records of an accuracy within 0.04 K per decade
646 (Ohring et al. 2005). The variability in the thickness, altitudes and temperatures of dust
647 layers can introduce additional uncertainties into comparisons between satellite- and M-
648 AERI-derived SST_{skin} . As the aerosol altitude increases, the SST_{skin} difference becomes
649 more negative, because higher dust layers have larger temperature contrasts to the sea
650 surface. Saharan dust layers present in the lower troposphere are usually accompanied
651 with high air temperatures, so the MODIS-derived SST_{skin} difference is likely to be
652 positive. The SST_{skin} differences due to aerosol vertical distributions can vary with
653 occasionally more extreme values between -3 K and 1 K.

654 Users seeking high-quality SSTs in areas where there is the risk of dust
655 contamination are encouraged to pay attention to the Quality Level indicator of each
656 pixel, and use the “best” quality data with QL=0. It should be noted that the MODIS
657 R2019 reprocessed SST_{skin} retrievals include a correction for dust effects at night, as
658 reported by Luo et al. (2019), but this correction does not take into account explicit
659 dependences on altitude, and hence temperature, and dust concentration.

660 The MODIS NLSST does not use measurements from infrared channels with
661 wavelengths close to 3.8 μm and 8.9 μm (GSFC 2020). As shown by Merchant et al.
662 (2006) and other subsequent studies (Le Borgne et al. 2013; Luo et al. 2019), the off-axis
663 characteristics of the brightness-temperature difference space of channels 20 ($\lambda = 3.8 \mu\text{m}$),
664 29 ($\lambda = 8.9 \mu\text{m}$), 31 ($\lambda = 11 \mu\text{m}$) and 32 ($\lambda = 12 \mu\text{m}$) can indicate the dust presence during
665 nighttime and would be helpful to improve the SST_{skin} retrieval.

666 This study focused on MODIS onboard TERRA but since the MODIS onboard
667 AQUA has consistent design and performance in terms of their spectral channels,
668 calibration stability and other characterizations (Xiong et al. 2009; Xiong et al. 2008b),
669 we expect similar results for Aqua MODIS SST_{skin} retrievals. Future work is planned to
670 include a scheme to reduce the infrared satellites SST_{skin} errors by accounting for the
671 vertical dust distribution. The measurements of aerosol vertical distributions and
672 properties resolved by the lidar on the Cloud–Aerosol Lidar Infrared Pathfinder Satellite
673 Observations (CALIPSO; Adams et al. (2012)) could be useful. Reanalysis data, such as
674 those data from MERRA-2 and ECMWF ERA5 (Hersbach et al. 2020), can provide
675 supplementary information when the CALIPSO data are not available. The solar and
676 satellite zenith angles were set to zero in this study so other zenith angles dependences

677 should be included in a future study. In the future, we may extend this study to newer
678 sensors such as VIIRS and ABI. Also, mineral dust effects in other regions, such as at
679 high latitudes where mineral dust lofted into the atmosphere (e.g. Dagsson-
680 Waldhauserova et al. (2019); Vogelmann et al. (2003); Willis et al. (2018)), will be
681 investigated.

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696 **Credit authorship contribution statement:**

697 Bingkun Luo: analysis; writing, review & editing; funding acquisition. Peter J.
698 Minnett: supervision, writing, review & editing; Nicholas R. Nalli: analysis; data
699 acquisition.

700 **Declaration of competing interest:**

701 The authors declare that they have no known competing financial interests or
702 personal relationships that could have appeared to influence the work reported in this
703 paper.

704

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