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1 Use of hyperspectral sounders to retrieve daytime sea-surface temperature 2 from mid-infrared radiances: Application to IASI

3
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9 10 **Highlights**

- 11 • SST retrievals using daytime spectra from the infrared hyperspectral sounder IASI
- 12 • Successful use of mid-infrared wavelengths despite large contributions of solar light.
- 13 • High consistency and accuracy of the temperatures retrieved from wavelengths between 3.6 to 4.0
14 μm .

15 16 **Keywords**

17 Sea surface skin temperature ; Infrared radiative transfer retrieval algorithm ; Infrared
18 Atmospheric Sounder Interferometer (IASI) ; Solar contribution ; Mid-infrared wavelengths

19
20 **Abstract:** We propose a physically-based methodology for sea-surface skin-temperature (SST)
21 retrievals from daytime spectra recorded by the hyperspectral Infrared Atmospheric Sounding
22 Interferometer (IASI). The approach, which takes sun light into account, minimizes the differences
23 between measured and computed radiances at numerous points within two windows centered near 3.7
24 and 4.0 μm . We demonstrate that, even when the solar contribution is large, with brightness
25 temperatures increased by several tens of kelvin at the shortest wavelengths, very consistent SSTs are
26 retrieved in both windows. Furthermore, the values obtained are, after correction for the cool-skin

27 effect, in excellent agreement (<0.05 K on average) with the in-situ measurements of the depth
28 temperature provided by nearby drifters. This opens renewed perspectives for daytime SST
29 determinations from space, since the IASI mid-infrared windows used here provide SSTs that are, with
30 respect to those retrieved around 9 and 11 μm , much less sensitive to errors in the computed radiative
31 contribution of water vapor.

32

33

34 **1. Introduction**

35 The importance of precisely knowing the sea-surface skin temperature (SST) and the efforts
36 made for its determination having been extensively discussed previously, the interested reader is
37 invited to consult e.g. (Robinson, 2010 ; Martin, 2014 ; Minnett et al., 2019). Recall that, in the
38 framework of climate monitoring, one needs to detect and quantify small regional or global SST
39 changes lower than 0.2 K/decade (see e.g. Ohring et al., 2005 ; Merchant et al., 2008 and 2012). For
40 that purpose, the key requirements for a climate SST record and the associated difficulties often
41 encountered, which have been discussed in detail in Capelle et al. (2022) and references therein, are:
42 (i) an accuracy < 0.1 K and a stability < 0.05 K/decade, (ii) a high homogeneity of long time series (15
43 years at minimum, for which assuring the continuity between sensors is often challenging), (iii) an
44 independency from any model or other SST product (such as in-situ measurements or other datasets)
45 and, finally, (iv) the highest achievable sensitivity to SST changes, the main difficulty being here to
46 correctly take into account the effects of the water vapor content of the atmosphere. Simultaneously
47 satisfying all these requirements is generally difficult, as it is the case for the majority of available SST
48 products which are derived using 2 or 3 wavelengths only, with retrieval algorithms generally based
49 on regressions from in-situ buoys or ships measurements, either in the infrared (AVHRR, MODIS,
50 etc..) or microwave (AMRS-E). In addition to the long term monitoring of the SST, another important
51 issue is to know the diurnal variations, a key information in a variety of contexts including the Diurnal
52 Temperature Range issue, remote sensing, ocean and climate modeling, and air-sea heat and gas fluxes
53 estimates (Stuart-Menteth et al., 2003 ; Bernie et al., 2007 ; Kawai and Wada, 2007 ; Clayson and
54 Bogdanoff, 2013 ; Morak-Bozzo et al., 2016 ; Ruzmaikin et al., 2017).

55 Within this framework, SST products derived from radiances collected by Earth-polar orbiting
56 satellites offer only a partial observation of the diurnal cycle due to their only two overpasses per day,
57 and to the fact that retrievals cannot be made under cloudy or dusty conditions for infrared sounders or
58 under heavy precipitation for microwave ones. However, they may provide reference inputs for the
59 improvement of climatic and oceanic models, since they complement the data provided by the buoys
60 network by offering a more complete spatio-temporal sampling (Merchant et al., 2019). Collocating
61 satellite observations with in-situ measurements at different local times may improve the modeling of

62 the diurnal variations of the near-surface thermal structure, but this requires an equal quality of the
63 SST restitution for both day- and night-time. This latter constraint is particularly challenging since
64 solar light may significantly contribute to mid-infrared radiances collected from space when looking
65 down to the surface, increasing observed brightness temperatures below 4 μm by several tens of
66 kelvin, as shown below and in Chen et al. (2013). Given the uncertainty in the modeling of the solar
67 contribution, this explains why practically all satellite-based daytime SST retrievals in the infrared use
68 radiances around 9-12 μm , even though the instrument provides data at shorter wavelengths (e.g.:
69 Walton et al., 1998 ; O'Carroll et al., 2012 ; Kilpatrick et al., 2015 ; Merchant et al., 2019 ; Minnett et
70 al., 2019). A good example is given by MODIS observations, with which nighttime SSTs are deduced
71 from measurements around 3.75, 3.96, 4.05, 11.0, and 12.0 μm , while only the last two wavelengths
72 are used in the treatment of daytime data (Kilpatrick et al., 2015). However recall the noticeable
73 exception of Merchant et al. (2009b) where the 11 and 3.9 μm channels were used to retrieve daytime
74 SSTs from the Geostationary Operational Environmental Satellite 12. In this study, the radiances for
75 the short wavelength were treated by removing, in order to obtain "pseudonighttime" data, the
76 associated solar contribution. The latter was computed in a way quite similar to that used in the present
77 study, but due to uncertainties on its prediction, only those measurements for which the solar photons
78 raise the brightness temperature by less than 1 K at 3.9 μm were retained (which is not the case in our
79 study, thanks to the availability of many mid-infrared channels in IASI spectra). Let us finally mention
80 a study (Liu et al., 2014) in which a method is proposed to remove the solar contribution from the data
81 at 3.7 μm provided by the Visible Infrared Imaging Radiometer Suite by using the radiances recorded
82 at 1.6 and 2.25 μm . Finally, it is important to recall that using only long wavelengths leads to a lower
83 accuracy of the SST retrieved from nighttime observations since the atmosphere is less transparent
84 around 10 μm than in the mid infrared, which induces errors principally linked to the water vapor
85 content of the atmosphere (Capelle et al., 2022). This is particularly important in regions with high
86 atmospheric humidity, as it is the case in Tropics [see e.g. (Merchant et al., 2009a) for AVHRR,
87 (Kilpatrick et al., 2015) for MODIS, (Embury et al., 2012) for AATSR, (Tsamalis and Saunders,
88 2018) for CCI ATSR SST].

89 In Capelle et al. (2022), we used nighttime observations from the Infrared Atmospheric
90 Sounding Interferometer, IASI (Hilton et al., 2012), in order to retrieve SSTs, using a physically-based
91 radiative-transfer model, from radiances within atmospheric-transparency windows. The main results
92 of that study, are threefold: (i) While systematic biases due to errors in the modeling of the radiative
93 contribution of water vapor (resulting from spectroscopic and/or atmospheric-state knowledge errors)
94 may significantly affect the SSTs retrieved around 9 and 11 μm (and to a lesser extent those at 4.7
95 μm), it is not the case for the windows centered at 3.7 and 4.0 μm . (ii) Despite the significant
96 radiometric noise at these short wavelengths of the IASI spectra (Serio et al., 2018), the latter provide
97 SSTs which are, after correction for the cool-skin effect [e.g. (Saunders, 1967 ; Fairall et al., 1996)], in
98 excellent agreement with nearby (in time and position) in-situ depth-temperature measurements, with
99 a mean difference lower than 0.05 K and a robust standard deviation of 0.25 K. (iii) The comparisons
100 made with in-situ measurements for the 2008-2020 Metop-A period have enabled to demonstrate the
101 excellent stability of the time series, with a trend of the satellite minus in-situ temperature difference
102 lower than 0.05 K/decade. The consistency between the three generations of IASI on-board Metop-A,
103 -B, and -C have also been verified by comparing their monthly-averaged $1^\circ \times 1^\circ$ grids SSTs over their
104 overlap periods (2013–2020 for Metop-A and Metop-B, and 2019–2020 for Metop-C), leading to a
105 mean SST difference lower than 0.02 K , with a SD of 0.3 K consistent with the natural variation of
106 the SST within a month. Altogether, these results satisfy the prerequisites enumerated above when
107 considering SST time series as a climate data record. This opens promising perspectives by
108 demonstrating the possibility to provide an accurate, as well as stable, SST time-series from IASI over
109 the planned 20 years of the Metops-suite, that will be followed by two more decades of the IASI-New
110 Generation missions (Crevoisier et al., 2014). Furthermore, these achievements and the discussion
111 made above show that and extension, beyond nighttime, of the study by Capelle et al. (2022) is
112 desirable and of interest.

113 This paper generalizes the study of Capelle et al. (2022) to IASI daytime near-nadir
114 observations by including the solar contribution in the radiative-transfer model. The main objective of
115 this methodology study is to demonstrate that, thanks to the availability of a large number of spectral
116 channels highly sensitive to surface temperature, the radiances around 3.7 and 4.0 μm enable accurate

117 SST determinations provided that the solar contribution is correctly taken into account. Recall that the
 118 IASI level2 SSTs are derived from an empirical orthogonal-function regression, using the principal
 119 component scores of the first two bands (August et al., 2012), disregarding the information brought by
 120 short wavelengths of the spectra. The theoretical model and input data used are presented in Sec. 2.
 121 The IASI spectra retained and the procedure for their analysis are the subjects of Sec. 3, the results
 122 being discussed in Sec. 4 before some concluding remarks (Sec. 5). Note that we here propose and
 123 validate a methodology and that analyses of SST long time series, as done in Capelle et al. (2022), is
 124 beyond the scope of the present paper.

125

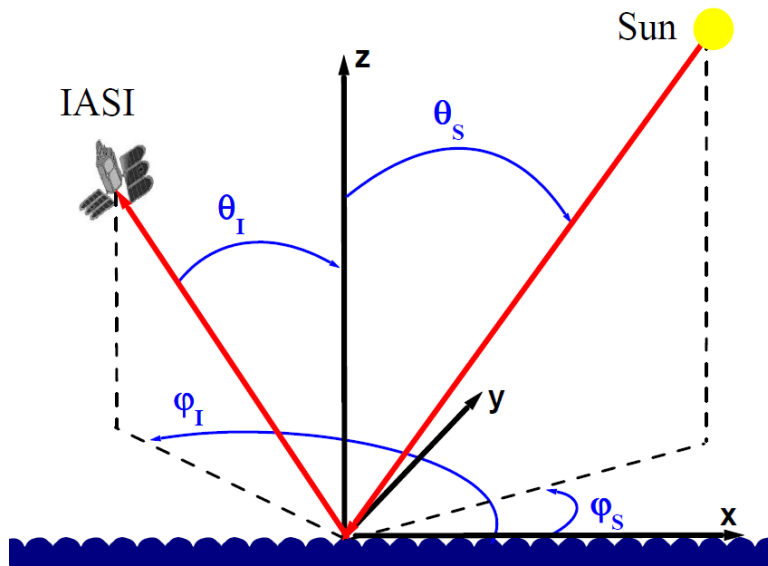
126 2. Theoretical model and data used

127 2.1 Theoretical model

128 For the observing geometry schematized in Fig. 1, the expression used to compute (and fit) the
 129 IASI radiance ($\text{W}/\text{m}^2/\text{str}/\text{cm}^{-1}$) at wave number σ (cm^{-1}) is:

$$130 \quad I_{\text{Theo}}(\sigma, \theta_I, \varphi_I, \theta_S, \varphi_S, T_{\text{Surf}}) = I_{\text{Surf}}(\sigma, \theta_I, T_{\text{Surf}}) + I_{\text{Atm_up}}(\sigma, \theta_I) \\
 131 \quad + I_{\text{Atm_down}}(\sigma, \theta_I) + I_{\text{Sun}}(\sigma, \theta_I, \varphi_I, \theta_S, \varphi_S) \quad (1)$$

131



132

133 **Fig. 1:** Observation geometry. The \vec{z} axis is along the local vertical, \vec{x} points toward the south and \vec{y} toward
 134 the east.

135

136 In this equation, which disregards any scattering of light in the atmosphere, the first term is the
137 emission by the surface transmitted up to the instrument. Assuming (see Sec. 2.2) that the sea-surface
138 directional emissivity $\varepsilon(\sigma, \theta_I)$ does not depend on the SST (T_{Surf}), and since both this emissivity and
139 the black-body radiance $I_{\text{BB}}(\sigma, T_{\text{Surf}})$ are constant over the narrow instrument function $F_{\text{Inst}}(\Delta\sigma)$ of
140 IASI, I_{Surf} is given by:

$$141 \quad I_{\text{Surf}}(\sigma, \theta_I, T_{\text{Surf}}) = \varepsilon(\sigma, \theta_I) \bar{\tau}(\sigma, \theta_I) I_{\text{BB}}(\sigma, T_{\text{Surf}}) , \quad (2)$$

142 with

$$143 \quad \bar{\tau}(\sigma, \theta_I) = \int_{-\infty}^{+\infty} F_{\text{Inst}}(\sigma - \sigma') \exp \left[- \int_0^{z_{\text{Inst}}} \alpha(\sigma', z) dz / \cos(\theta_I) \right] d\sigma' , \quad (3)$$

144 where z_{Inst} is the altitude of IASI, and $\alpha(\sigma, z)$ denotes the atmospheric absorption coefficient at
145 altitude z .

146 Using the same notations, the second term in Eq. (1), representing the emission of the atmospheric
147 column between the surface and the instrument, is given by:

$$148 \quad I_{\text{Atm_up}}(\sigma, \theta_I) = \int_{-\infty}^{+\infty} F_{\text{Inst}}(\sigma - \sigma') \int_0^{z_{\text{Inst}}} I_{\text{Loc}}(\sigma', z, \theta_I) dz / \cos(\theta_I) d\sigma' , \quad (4)$$

149 with

$$150 \quad I_{\text{Loc}}(\sigma', z, \theta_I) = I_{\text{BB}}[\sigma', T(z)] \alpha(\sigma', z) \exp \left[- \int_z^{z_{\text{Inst}}} \alpha(\sigma', z') dz' / \cos(\theta_I) \right] . \quad (5)$$

151 The third term in Eq. (1) is the emission of the atmosphere toward the surface that is then reflected and
152 transmitted up to the instrument. Rigorously speaking, it involves an integration over all possible
153 downward-emission directions, each weighted by the proper (which ensures that the considered light is
154 redirected within the IASI field of view) bi-directional reflectivity. Since the probability of the latter
155 depends on the wind-dependent wave-slope distribution and because an angular integration must be
156 made, a correct calculation of $I_{\text{Atm_down}}(\sigma, \theta_I)$ for each treated IASI spectrum is extremely costly. In
157 order to avoid doing so, we first carried simplified calculations corresponding to the extreme cases of
158 Lambertian and specular reflectances, respectively [note that these are close to the limit cases of the
159 sea surface for very high and low wind conditions, respectively (Watts et al., 1996)], and treated a

160 limited but representative set of IASI spectra. The first case can be correctly predicted by considering
 161 a single path with an elevation angle of $\theta_{\text{down}} = 53^\circ$ (Turner, 2004), while the second also considers a
 162 single elevation angle $\theta_{\text{down}} = \theta_I$, now identical to that of the IASI pointing. One thus has:

$$163 \quad I_{\text{Atm_down}}(\sigma, \theta_I) = \int_{-\infty}^{+\infty} F_{\text{Inst}}(\sigma - \sigma') \int_0^{+\infty} I_{\text{Loc}}(\sigma', z, \theta_{\text{down}}) dz / \cos(\theta_{\text{down}}) d\sigma', \quad (6)$$

164 with

$$165 \quad I_{\text{Loc}}(\sigma', z, \theta_{\text{down}}) = [1 - \varepsilon(\sigma', \theta_I)] \exp\left[-\int_0^z \alpha(\sigma', z') dz' / \cos(\theta_I)\right] \\ \times I_{\text{BB}}[\sigma', T(z)] \alpha(\sigma', z) \exp\left[-\int_0^z \alpha(\sigma', z') dz' / \cos(\theta_{\text{down}})\right]. \quad (7)$$

166 The results of our tests show that the mean difference between the SSTs obtained using the specular
 167 and Lambertian assumptions is of typically +0.025 K, a weak difference which could be expected
 168 from the smallness of both the atmospheric absorption and sea water reflectance, regardless of the
 169 water vapor content of the involved atmosphere. Considering that this value is ten times smaller than
 170 the standard deviation, that using the fixed value $\theta_{\text{down}} = 53^\circ$ independently of the IASI pointing is
 171 technically simpler, and by consistency with what was done in the analysis of nighttime spectra
 172 (Cappelle et al., 2022), we have retained this choice for the final processing of all the spectra.

173 Finally, the solar contribution, $I_{\text{Sun}}(\sigma, \theta_I, \varphi_I, \theta_S, \varphi_S)$, is written as:

$$174 \quad I_{\text{Sun}}(\sigma, \theta_I, \varphi_I, \theta_S, \varphi_S) = A(\theta_I, \varphi_I, \theta_S, \varphi_S) \rho(\sigma, \theta_I, \varphi_I, \theta_S, \varphi_S) \cos(\theta_S) d\Omega_S \\ \times \int_{-\infty}^{+\infty} F_{\text{Inst}}(\sigma - \sigma') I_{\text{Sun}}^0(\sigma') \exp\left[-\int_0^z \alpha(\sigma', z) dz / \cos(\theta_I)\right] \exp\left[-\int_0^{+\infty} \alpha(\sigma', z) dz / \cos(\theta_S)\right] d\sigma', \quad (8)$$

175 where $I_{\text{Sun}}^0(\sigma)$, $d\Omega_S$, and $\rho(\sigma, \theta_I, \varphi_I, \theta_S, \varphi_S)$ respectively denote the (disk-averaged) radiance
 176 emitted by the sun, the solid angle within which the sun is seen from Earth, and the bi-directional
 177 spectral reflectivity of the surface. The factor $A(\theta_I, \varphi_I, \theta_S, \varphi_S)$ includes the probability for waves to
 178 have a slope enabling solar photons coming along the (θ_S, φ_S) direction to be redirected toward the
 179 instrument (along θ_I, φ_I) after a specular reflection. Its value can be computed (as discussed in Sec.
 180 4.1) from knowledge of the observation geometry and of the wind direction and speed. However, since
 181 its prediction carries uncertainties (Zhang and Wang, 2010 ; Liang et al., 2010) that may bias the

182 retrieved SSTs, this quantity is below considered as an unknown to be fitted in the analysis of the
183 spectra.

184 Most of the terms participating to Eqs. (1)-(8) can be computed from knowledge of the sea water
185 optical constants, as well as of the thermodynamic conditions of each observed scene (i.e. the vertical
186 profiles of temperature, pressure, ...), and molecular absorption data feeding the calculation of the
187 absorption coefficient. Since all these input data can be determined upstream independently (see Sec.
188 2.2), the theoretical radiance thus involves two unknowns only: $A(\theta_I, \varphi_I, \theta_S, \varphi_S)$, through $I_{\text{Sun}}(\dots)$ in
189 Eq. (8), and T_{Surf} , through $I_{\text{BB}}(\sigma, T_{\text{Surf}})$ in Eq. (2). Their values were retrieved from fits of IASI
190 spectra as explained in Sec. 3.2.

191

192 **2.2 Input data and computational tools used.**

193 The sea-surface emissivity $\varepsilon(\sigma, \theta_I)$ was computed, following Masuda et al. (1988), using the
194 complex index of refraction for pure water of Downing and Williams (1975), after a shifting of $+4\text{cm}^{-1}$
195 and an increase of the real part by $+6 \cdot 10^{-3}$ (Friedman, 1969) in order to take salinity effects into
196 account. The small (Newman et al., 2005 ; Masuda, 2008), or unknown, dependence of $\varepsilon(\sigma, \theta_I)$ on the
197 SST was disregarded and, since we consider observations close to nadir ($|\theta_I| < 30^\circ$), the weak (Masuda
198 et al., 1988) influence of the wind speed was neglected. The reflectivity $\rho(\sigma, \theta_I, \varphi_I, \theta_S, \varphi_S)$ was
199 computed (see Appendix A) using Fresnel's coefficients, Snell's law, and the complex index of
200 refraction mentioned above. In the 3.6 to 4.0 μm region used for the final retrievals, the solar radiance
201 was represented by a Planck function with a temperature of 5657 K compatible with Platnick and
202 Fontenla (2008). Note that the sensitivities of the results to the index of refraction and solar spectrum
203 are discussed in Appendix B which also validates the input data retained. As done by Capelle et al.
204 (2022) and Hartmann et al. (2018), the absorption coefficients were computed, for each atmospheric
205 state (see below), using the 4AOP code (Scott and Chédin, 1981 ; Cheruy et al., 1995). The
206 spectroscopic parameters for the individual lines of absorbing gases were taken from the GEISA
207 database (Jacquinet-Husson et al., 2016), complemented by the MT_CKD (version 3.1)
208 parameterization (Mlawer et al., 2012) of the water-vapor continuum, and the collision-induced

209 absorption by N₂ as well as CO₂ line-wing corrections were implemented as in Hartmann et al. (2018).
210 Local Thermodynamic Equilibrium (LTE) was assumed, an approximation which breaks down for the
211 populations of some molecular vibrational levels at elevated altitude (López-Puertas and Taylor,
212 2001). However, non-LTE only affects the atmospheric emission close to the centers of intense
213 absorption bands [e.g. near 4.3 μm for CO₂ (DeSouza-Machado et al., 2007 ; Chen et al., 2013)],
214 regions disregarded in the present study which, contrariwise, uses transparency windows where the
215 atmospheric transmission is high (see Sec. 3.2).

216 The calculations of the atmospheric absorptions, transmissions and emissions require
217 knowledge of the altitude-dependent state (temperature, pressure, volume mixing ratios of the
218 absorbing species) of the atmosphere probed by each IASI observation. Here, the temperature and
219 water profiles are determined independently, as in Capelle et al. (2022), using a proximity recognition
220 in brightness temperature (BT) within the Thermodynamic Initial Guess Retrieval (TIGR)
221 climatological database (Chédin et al., 1985 ; Chevallier et al., 1998). For all of the atmospheric
222 situations in TIGR, BTs are computed with the radiative transfer model (4A/OP) for a set of 8
223 channels, carefully selected principally in the 13-14 μm spectral band, and then compared with the
224 corresponding observed IASI BTs. The channels used are principally sensitive to the temperature and
225 water profiles with relatively small contributions from other gases, the surface or the sun [see also
226 (Capelle et al., 2012) for a complete description].

227 The wind speed and direction needed for the calculation of the solar parameter A come from
228 interpolation of the hourly 0.25°x0.25° resolution European Centre for Medium-Range Weather
229 Forecasts' (ECMWF) 5th Re-Analysis (ERA5) dataset (Hersbach and Dee, 2016).

230

231 **3. The IASI spectra and their treatment**

232 **3.1 Selected IASI spectra**

233 In order to validate the methodology proposed in this paper, a limited but nonetheless
234 sufficiently large set of 99010 IASI Metop-A daytime observations was used. These spectra, recorded
235 between 2015 and 2019, were selected using the following criteria: (i) Only cloud- and aerosol-free

236 observations were retained, selected by using criteria on brightness temperatures from IASI and the
237 collocated AVHRR instrument, as explained in Capelle et al. (2022). As in this latter study, the largest
238 dust-contaminated observations that may remain after the cloud-aerosol filtering are removed by
239 retrieving the dust optical depth (DAOD) at 10 μm using the method described in Capelle et al. (2018).
240 For nighttime spectra, every observation with a DAOD>0.03 was eliminated in Cappelle et al. (2022).
241 For daytime observations, to avoid any contamination by the solar contribution in the DAOD
242 retrievals (which is based on the use of channels not only in the range 8-12 μm , but also around 4.7
243 μm), only the observations with a DAOD>0.2 are eliminated. These limit values have been chosen
244 empirically. (ii) We only kept those IASI spectra for which an in-situ depth-temperature measurement,
245 made from a drifter close to the observed sea spot in both localization (< 20 km away) and time (< 3 h
246 difference, 98.8% of them being within 1 h difference), is available from the NOAA in-situ Quality
247 Monitor (IQUAM; <https://www.star.nesdis.noaa.gov/socd/sst/iquam/>) (Xu and Ignatov, 2014). (iii)
248 Data collected for $|\theta_1|>30^\circ$ were disregarded in order to minimize potential biases resulting from the
249 dependence of the sea-surface emissivity on wind speed (Masuda et al., 1988). Note that the selected
250 set includes recordings made for a large variety of atmospheric-humidity conditions, with total
251 precipitable water contents between 0.2 and 6.7 cm.

252

253 **3.2 Analysis procedure**

254 In the treatment of the observations, some of the spectral channels of locally minimum
255 absorption selected by Capelle et al. (2022) were used. We here only retained the two windows of
256 highest frequencies: W₄, with 107 points from 2480 to 2528 cm^{-1} and W₅, with 185 points from 2594
257 to 2760 cm^{-1} . Following the conclusions of Capelle et al. (2022), the longer wavelengths (W₁ around
258 11 μm ; W₂ around 9.0 μm ; W₃ around 4.7 μm) were not used given their too large sensitivities to
259 errors in the computation of the (poorly known) contribution of water vapor as well as in the sea-
260 surface emissivity and atmospheric temperature profile. These sensitivities, analyzed in Appendix A of
261 Capelle et al. (2022), result from the larger contribution of the water vapor continuum and weaker

262 dependence of the blackbody function on temperature at long wavelengths when compared to short
263 ones. The analysis of each spectrum used three steps.

264 Step 1: The retained measured radiances were simultaneously fitted using Eqs. (1)-(8), floating
265 $A(\theta_I, \varphi_I, \theta_S, \varphi_S)$ and \bar{T}_{Surf} in order to minimize the mean deviation, over all channels inside
266 windows W_4 and W_5 , between the measured and computed radiances, i.e. the quantity:
267 $\sum_{\sigma_i \in W_4 \& W_5} [I_{\text{Theo}}(\sigma_i, A, \bar{T}_{\text{Surf}}) - I_{\text{IASI}}(\sigma_i)]^2$. It is important to emphasize that this procedure is
268 made possible by the hyperspectral character of IASI [which is not the case for MODIS (Kilpatrick et
269 al., 2015) and GOES-12 (Merchant et al., 2009), for instance] and the associated availability of
270 numerous channels in a wavelength region over which the solar spectrum shows important relative
271 variations and may significantly contribute to the measured radiances.

272 Step 2: The value of $A(\theta_I, \varphi_I, \theta_S, \varphi_S)$ was then fixed, and $T_{\text{Surf}}(\sigma_i)$ was retrieved, for all selected
273 channels σ_i , by solving the equation $I_{\text{Theo}}[\sigma_i, A, T_{\text{Surf}}(\sigma_i)] = I_{\text{IASI}}(\sigma_i)$. Setting A to zero in this
274 exercise yields SST values “as if it were nighttime” since the solar photons collected by the instrument
275 are then disregarded. For a preliminary test of steps 1 and 2, we selected a spectrum showing a
276 significant solar contribution and collected over a dry atmosphere, and used all the (five) windows
277 retained for the treatment of nighttime observations (Capelle et al., 2022). Figure 2 exemplifies the
278 results obtained and shows that, for the analyzed observation, the effect of solar light is obvious in W_4
279 and W_5 while it is negligible in W_1 and W_2 , a result explained by the fact that $I_{\text{Sun}}^0(\sigma)/I_{\text{BB}}(\sigma, T_{\text{Surf}})$
280 increases exponentially with σ and varies by more than three orders of magnitude from the lowest
281 ($\sim 830 \text{ cm}^{-1}$) to the highest ($\sim 2760 \text{ cm}^{-1}$) wave number. Figure 2 also demonstrates that, in contrast to
282 the treatment disregarding sun light (using $A=0$), taking the latter into account provides SSTs that are
283 consistent throughout the entire spectral range. Note that the increase of the IASI noise with σ (Serio
284 et al., 2018) is responsible for the corresponding increase of the scatter of $T_{\text{Surf}}(\sigma)$, an effect further
285 amplified when the sun contribution is large. Indeed, in the case of Fig. 2, the radiance due to solar
286 photons represents, near 2600 cm^{-1} , more than half of the signal collected by IASI which, after its

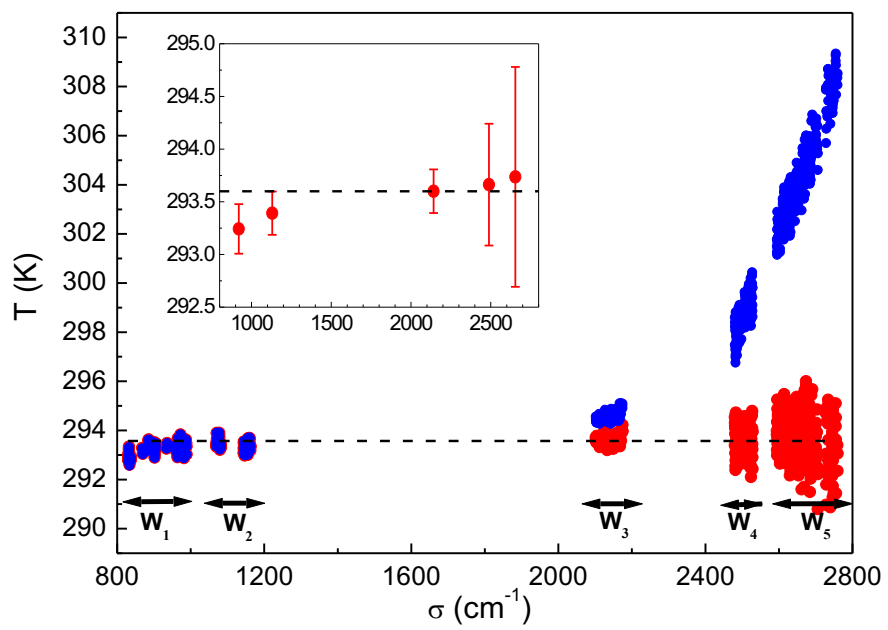
287 removal, increases the scatter of $T_{\text{Surf}}(\sigma_i)$ by a factor of about two, explaining the greater dispersion
 288 of the red points when compared to the blue ones.

289 Step 3: Finally, for the further analyses of the consistency of the SSTs retrieved in different spectral
 290 windows W_k , we from now on consider the averages:

$$291 \quad \bar{T}_k = \bar{T}_{\text{Surf}}(W_k) = \sum_{\sigma_i \in W_k} T_{\text{Surf}}(\sigma_i) / N_k, \quad (9)$$

292 where N_k is the number of data points inside W_k (see example in the insert of Fig. 2).

293



294
 295 **Fig. 2:** Main panel: SSTs retrieved by taking into account (red circles) and disregarding (blue circles) the solar
 296 contribution. The horizontal dashed line represents the average of all red circles. Insert: Averages, \bar{T}_k [see Eq.
 297 (9)], of the temperatures $T_{\text{Surf}}(\sigma_i)$ retrieved in each window W_k by taking the solar light into account (the error
 298 bars represent the standard deviation), the horizontal dashed line denoting the uncertainty-weighted average.

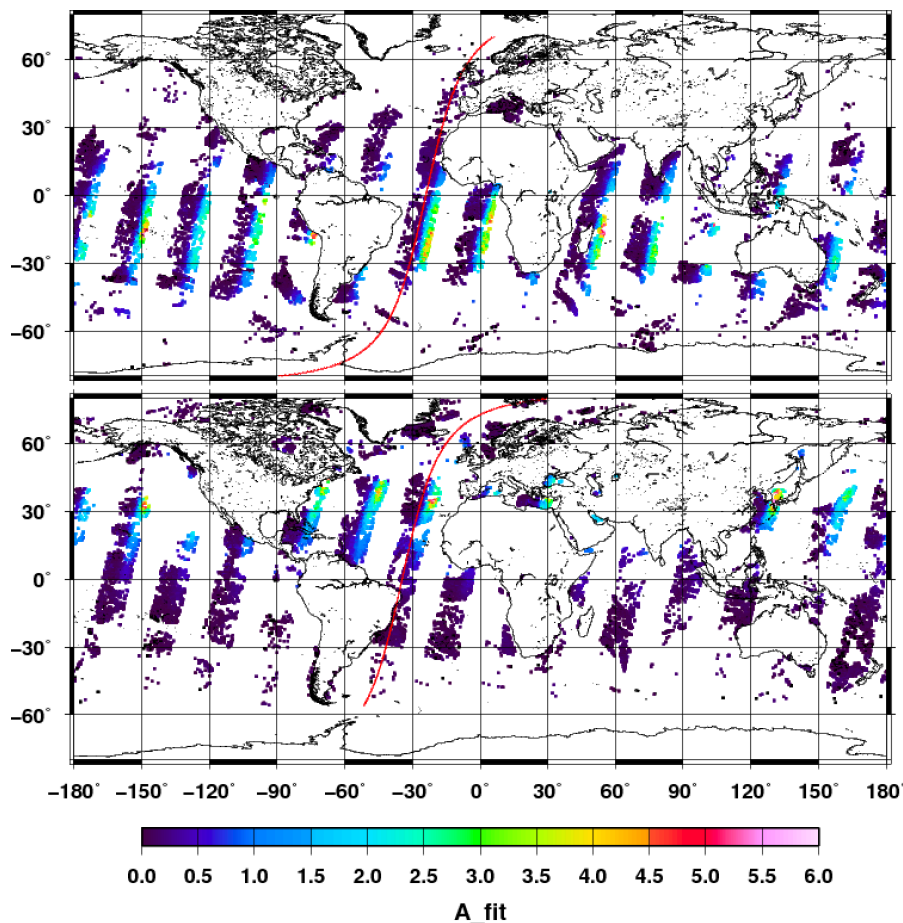
299

300 4. Results and discussion

301 4.1 The solar parameter A

302 In many of the observations the solar contribution, and thus also the retrieved A_{Fit} parameter,
 303 is small, except when the instrument points close to the sun glint which, for the geometry of Fig. 1,

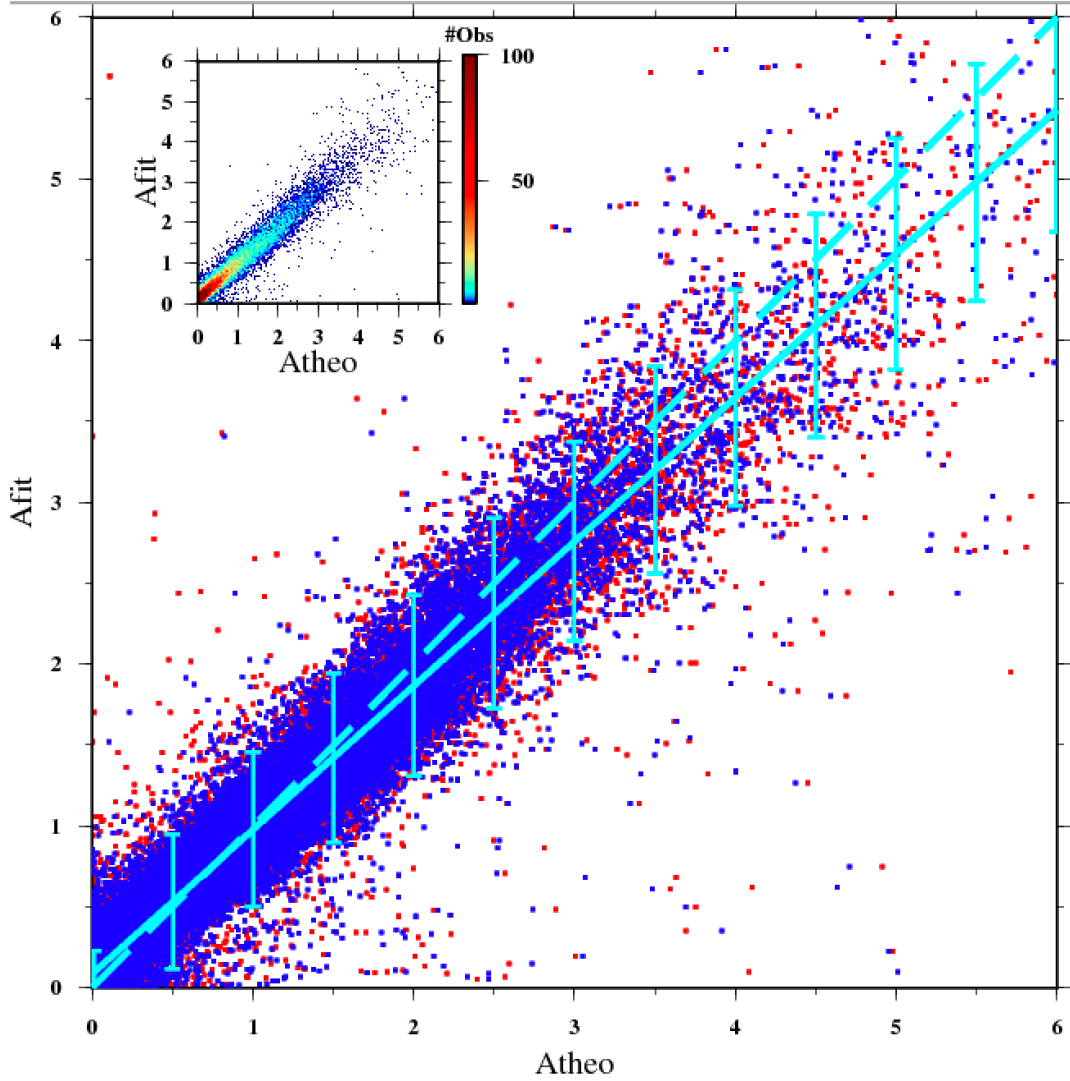
304 corresponds to small values of both $\theta_I - \theta_S$ and $\varphi_I - \varphi_S$. Since the IASI orbits are close to the South-
 305 North axis, the swath practically follows the East-West direction and, for the retained observations
 306 close to nadir, θ_I hence varies between 0° and 30° while φ_I is close to 90° (Eastward pointing) or
 307 270° (Westward pointing). The local time of all observations being 9:30 AM at the Equator, the sun is
 308 in the East, implying that a large solar contribution may only be collected on this side of the swath and
 309 when the sun azimuth angle φ_S is close to 90° . According to this last criterion, large values of A_{Fit}
 310 will be obtained during the winter at moderate south latitudes only, because the sun inclination to the
 311 South is too large (i.e. φ_S is significantly smaller than 90°) in the Northern hemisphere, the situation
 312 being reversed in the summer. All these considerations are confirmed by the maps in Fig. 3, which
 313 corresponds to the orbits of July 16 and January 25 in 2018.



314
 315 **Fig. 3:** Color maps of the values of the solar parameter retrieved from the IASI spectra collected along the 2018
 316 orbits of January 25 (top panel) and July 16 (lower panel). The red line on the central orbits indicates the
 317 center of the swath (nadir pointing).

318

319 Now, before discussing the SSTs, a first validation of the proposed methodology is performed
320 by assessing the quality of the retrieved solar parameter by comparison with predictions based on two
321 parameterizations of the probability of wave slopes (Cox and Munk, 1954 ; Bréon and Henriot, 2006)
322 calculated from knowledge of the geometry of the observation and of the wind direction and speed
323 (see Appendix C). The fitted (A_{Fit}) and theoretical (A_{Theo}) values for every IASI observation treated in
324 this study are compared in Fig. 4 (where 99.45% of the points satisfy $|A_{\text{Fit}}-A_{\text{Theo}}|\leq 1$). Note that, in
325 this plot, we have retained only those results associated with observations for which the wave-tilt
326 angle θ_W [see Eq. (A8) of Appendix C] is smaller than 25° since this is the limit of reliability of the
327 above mentioned models. As can be seen, the retrieved and predicted values are very consistent, the
328 best linear fit of the data in Fig. 4 leading (with close results for the two models of A_{Theo}) to a slope of
329 0.9, an offset of 0.09, and a correlation value of 0.97. The insert, displaying the corresponding scatter
330 density plot obtained for the parametrization of (Bréon and Henriot, 2006), indicates that the
331 maximum of density is centered on the best linear fit, with the majority of situations corresponding to
332 small values of A_{Theo} (as it can be expected from Fig. 3) The density plot for the parametrization of
333 (Cox and Munk, 1954) gives a similar pattern (not shown). Furthermore, the deviations with respect to
334 $A_{\text{Fit}}=A_{\text{Theo}}$ are practically within the combined uncertainties of our determinations, indicated by error
335 bars on the plot, and of the theoretical models, estimated from the uncertainties on the wave-slope
336 probability-law parameters given by Cox and Munk (1954) and Bréon and Henriot (2006) as being
337 about 0.2 and 0.08, respectively. These results provide a first validation of the procedure proposed
338 here. Note that, although the blue symbols in Fig. 4 seem slightly less scattered than the red ones,
339 concluding that the most recent facet model (Bréon and Henriot, 2006) would be the best remains
340 hazardous due to uncertainties and to the limited number of observations (about 10^5) considered here.
341 Furthermore recall that the comparisons in Fig. 4 are only presented for a first validation of our
342 method and that the present paper focuses on its test from the point of view of the SST. An evaluation
343 of the wave-slope models is thus beyond the scope of this study, but this issue is currently under
344 investigation and will be adressed in a forthcoming study considering much more IASI observations.



345

346

347 **Fig. 4:** Comparison between the A_{Fit} parameters obtained from fits of IASI spectra with those, A_{Theo} , calculated
 348 (see Appendix C) for each observation (provided that the wave-tilt angle is smaller than 25°) by using the
 349 parameterizations of Cox and Munk (1954) (red circles) and of Bréon and Henriot (2006) (blue circles), and the
 350 wind speed and direction provided by ECMWF (see Sec. 2.2 and Appendix C). The cyan error bars on A_{Fit}
 351 represent the one sigma statistical one from the least-square fit. The full and dashed cyan lines represent the best
 352 linear fit and the $A_{Fit}=A_{Theo}$ law, respectively. Insert: corresponding scatter density plot for boxes of 0.03×0.03
 353 obtained for the parameterizations of Bréon and Henriot (2006).

354

355 4.2 The SSTs

356 We now focus on the validation of the retrieved sea-surface (skin) temperatures. For that
 357 purpose, the averaged values \bar{T}_4 and \bar{T}_5 [Eq. (9)] obtained from the 3.7 and 4.0 windows are

358 compared with in-situ measurements from drifters (Sec. 3.1). The latter provide the “depth
359 temperature” T_{Depth} , measured typically 20 cm below the surface, while $\bar{T}_{k=4,5}$ are representative of
360 the “skin temperature” T_{Skin} , corresponding to few micrometers below the surface. In order to directly
361 compare them, a model representing their theoretical differences ($\Delta T = T_{\text{Skin}} - T_{\text{Depth}}$) is thus needed.
362 During night, a “cool-skin effect” around -0.2 K is observed and predicted (Saunders, 1967 ; Fairall et
363 al., 1996 ; Donlon et al., 2002 ; Minnett et al., 2011), which was taken into account in Capelle et al.
364 (2022) using the approach proposed by Fairall et al. (1996), forced by the surface fluxes and the
365 friction velocity provided by the European Centre for Medium-Range Weather Forecasts (ECMWF)
366 model ERA5 forecast data (Hersbach et al., 2018 and 2020) with sea-water thermophysical properties
367 from web.mit.edu/seawater (Sharqawy et al., 2010; Nayar et al., 2016). During the day, this effect is
368 slightly reduced by the heating due to the absorption of a portion of the solar flux within the ocean
369 skin layer. In order to compute ΔT , we used Eq. (14) of Fairall et al. (1996), updated as described by
370 Wick et al. (2005). Finally, under slow-wind conditions, the solar heating may also induce a warming
371 that decreases with depth but may be significant near the surface, leading to a thermal stratification in
372 the upper layer of the ocean. This effect was taken into account using the simple parameterization
373 described in Zeng and Beljaars (2005). Altogether, the skin-to-depth corrections used here are similar
374 to those applied in the ECMWF model and described in (ECMWF, 2016). It must be emphasized that
375 these parameterizations are not exact, a statement which particularly applies to that of the warm layer
376 since it is based on a too simple thermal stratification. In addition, they depend on ERA5 surface
377 fluxes, which are not observations, but models. The skin-to-depth conversion is therefore not
378 expected to be fully accurate, in particular for slow wind and high insolation conditions, where the
379 warm layer effect is not negligible.

380 In the following, statistics for the differences $\Delta T_5 \equiv \bar{T}_5 - T_{\text{Depth}}$ obtained from IASI spectra in
381 window W_5 are discussed, expressed in terms of the median (M) and robust standard deviation (RSD),
382 defined as 1.5 times the Median Absolute Deviation, i.e. the median of all the absolute difference
383 between each individuals points and the median of the population (e.g. Rousseeuw and Hubert, 2011),
384 instead of the mean (Mean) and standard deviation (STD), as often done in SST analyses, in order to

385 attenuate the effect of outliers due to unscreened clouds or to errors in the measurement [see (Capelle
386 et al., 2022) and references therein]. They are complemented by considering the double difference
387 $\delta\Delta T_5 \equiv \Delta T_5 - \Delta T_{\text{Theo}}$, where ΔT_{Theo} denotes the value of the skin-to-depth temperature difference
388 computed for each observation as explained above, all the results, including those for ΔT_4 and $\delta\Delta T_4$,
389 being summarized in Table 1 where the nighttime results from Capelle et al. (2022) are recalled.
390

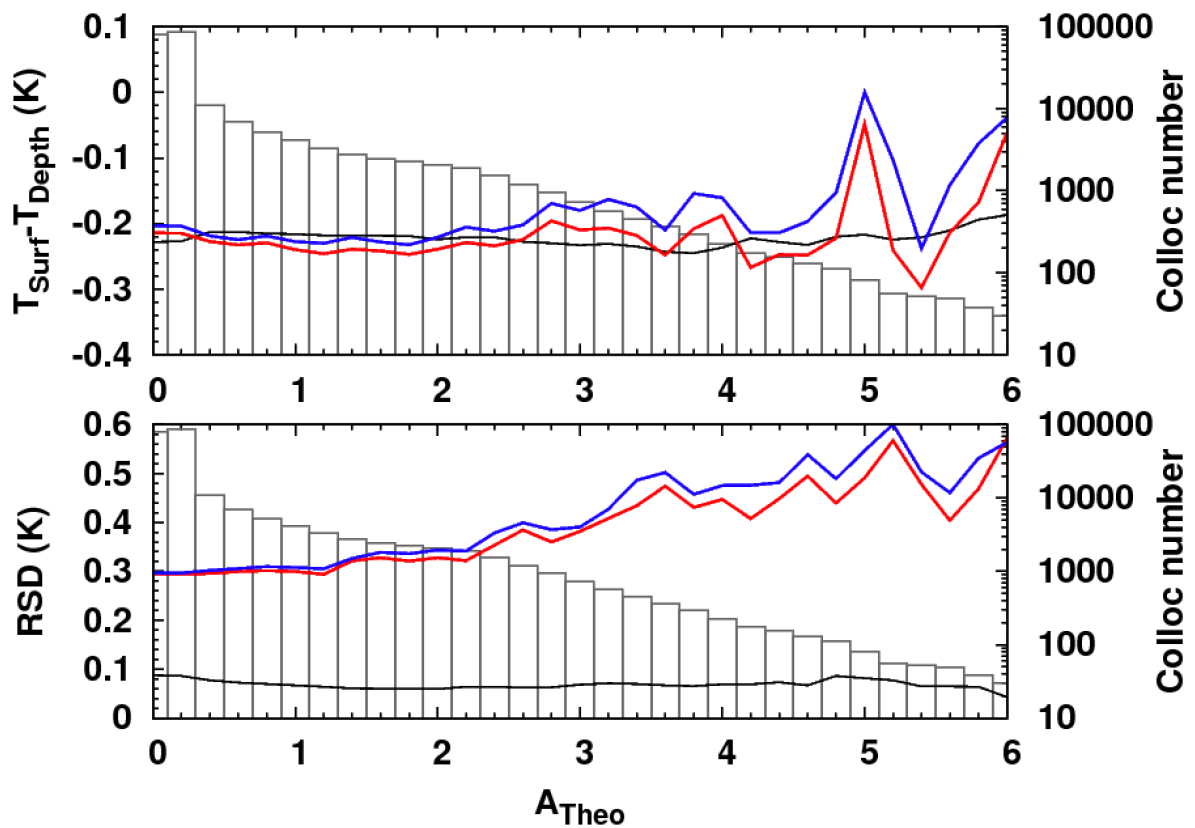
	All colloc (99010)				$A_{\text{Theo}} < 0.5$ (81458 colloc)				$A_{\text{Theo}} > 1$ (11060 colloc)			
	ΔT_k (K)		$\delta\Delta T_k$ (K)		ΔT_k (K)		$\delta\Delta T_k$ (K)		ΔT_k (K)		$\delta\Delta T_k$ (K)	
	k=4	k=5	k=4	k=5	k=4	k=5	k=4	k=5	k=4	k=5	k=4	k=5
Mean	-0.21	-0.22	0.01	0.00	-0.21	-0.22	0.02	0.00	-0.22	-0.24	0.00	-0.02
	-0.25	-0.28	0.00	-0.02								
STD	0.37	0.36	0.37	0.36	0.37	0.36	0.36	0.36	0.40	0.38	0.39	0.38
	0.37	0.37	0.37	0.38								
Median	-0.20	-0.21	0.03	0.02	-0.20	-0.21	0.03	0.02	-0.21	-0.23	0.01	-0.01
	-0.23	-0.26	0.02	-0.01								
RSD	0.30	0.30	0.30	0.30	0.30	0.29	0.29	0.29	0.35	0.34	0.35	0.33
	0.25	0.24	0.25	0.25								

391
392 **Table 1:** Statistics of the IASI (skin) versus in-situ drifter (depth) temperature differences in windows $W_{k=4}$
393 (around 4.0 μm) and $W_{k=5}$ (around 3.7 μm). $\Delta T_k \equiv \bar{T}_k - T_{\text{Depth}}$ is the difference between the retrieved
394 temperature \bar{T}_k and the collocated in-situ measured depth temperature T_{Depth} , while
395 $\delta\Delta T_k \equiv \Delta T_k - \Delta T_{\text{Theo}}$, where ΔT_{Theo} denotes the value of the skin-to-depth temperature difference
396 computed for each observation, as explained in Sec. 4.2, following Fairall et al. (1996), Wick et al.
397 (2005) and Zeng and Beljaars (2005). The numbers in bold characters in columns 2 to 5 correspond to
398 the nighttime results for the same period from Capelle et al. (2022).

399

400 The overall median temperature difference ΔT_5 obtained between IASI and the drifters for the 99010
401 collocations analyzed in the W_5 window is $M(\Delta T_5)=-0.21$ K ($RSD=0.30$ K). After correction of the
402 cool-skin effect as explained above, the corresponding values for $\delta\Delta T_5=\Delta T_5 -\Delta T_{\text{Theo}}$ are $M(\delta\Delta T_5)=0.02$
403 K ($RSD=0.30$ K). These results are close to those obtained, for the same time period, from nighttime
404 observations by Capelle et al. (2022), i.e. $M(\Delta T_{15})=-0.26$ K ($RSD=0.24$ K) and $M(\delta\Delta T_5)=-0.01$ K
405 ($RSD=0.25$ K), respectively. As already observed for nighttime observations in Capelle et al. (2022),
406 $M(\Delta T_{\text{IASI}})$ is slightly larger than the average value generally retained for skin-to-depth temperature
407 conversion (e.g. $\Delta T=-0.17$ K in Donlon et al. (2002); $\Delta T=-0.13$ K in Minnett et al. (2011). However,
408 it should be emphasized that these last two numbers, obtained from shipboard measurements,
409 correspond to an asymptotic behavior reached for wind speeds larger than $8 \text{ m}\cdot\text{s}^{-1}$, which is not
410 representative of the majority of the observations used here. For the collocations analyzed here, the
411 averaged wind speed is $6 \text{ m}\cdot\text{s}^{-1}$, and the resulting observed depth-to-skin effect of -0.21 K is, for this
412 wind speed value, in agreement with the above mentioned studies. However, these overall statistics
413 include SSTs retrieved for observations involving a broad range of solar contributions, with spectra
414 which are close to nighttime conditions, when the instrument looks in a direction opposite to that of
415 the sun, and others that are largely affected, when the instrument points near the sun glint (see Fig. 3).
416 In order to evaluate the robustness of our procedure when the sun contribution increases, we display,
417 in Fig. 5, the evolution of the median ΔT s retrieved in windows W_4 and W_5 versus the solar parameter
418 A_{Theo} , since the latter is well adapted for this purpose. This statement is demonstrated by Fig. A2 of
419 Appendix D, where the impact of the solar contribution on the retrieved temperature \bar{T}_5 (i.e. the
420 difference between the value obtained using the fitted parameter A_{Fit} and that retrieved imposing
421 $A_{\text{Fit}}=0$) shows a strong correlation with A_{Theo} . Note that Fig. A2 also points out the potential large
422 impact of the sun on the temperature retrieval, with errors higher than 40 K when solar photons are
423 disregarded. Figure 5 shows that: (i) the retrieved ΔT s are extremely stable with A_{Theo} , with an almost
424 constant value around -0.2 K ; (ii) the values obtained using the W_4 and W_5 windows are very
425 consistent, even if their difference slightly increases with the magnitude of the solar contribution ; (iii)

426 the ΔT s obtained from IASI spectra are in excellent agreement with the skin-to-depth temperature
 427 differences computed as described above, implying that the absolute bias in our retrieval is very small
 428 and stable whatever the magnitude of the solar contribution. For instance, the difference between the
 429 IASI-retrieved ΔT in window W_5 and the theoretical predictions has a median $M(\delta\Delta T_5) = 0.02$ K
 430 ($RSD = 0.29$ K) for observations with a very small solar contribution ($A_{\text{Theo}} < 0.5$), while $M(\delta\Delta T_5) = -0.01$
 431 K ($RSD = 0.33$ K) when spectra significantly affected by the sun ($A_{\text{Theo}} > 1.0$) are used (similar values are
 432 obtained for W_4 as shown by Table 1). Recalling that neglecting solar light leads (see Fig. A2 of
 433 Appendix D) to errors on \bar{T}_5 that vary from negligible to about 40 K along the x axis of Fig. 5, these
 434 result demonstrate the extreme robustness of the retrieval procedure proposed in this paper. It is worth
 435 noting that the SSTs obtained here from sun-contaminated spectra have, as those retrieved from
 436 nighttime observations (Capelle et al., 2022), absolute biases below the 0.1 K threshold required
 437 (Ohring et al., 2005 ; Merchant et al., 2008 ; Minnett and Corlett, 2012) for a SST product usable for
 438 climate studies.



439

440

441 **Fig. 5:** Upper panel: Left y axes: Average (over all observations using a bin of $\Delta A_{\text{Theo}}=0.2$) differences
442 $\Delta T_k = \bar{T}_k - T_{\text{Depth}}$ between the sea-surface skin temperatures \bar{T}_4 and \bar{T}_5 retrieved from IASI spectra in windows
443 W_4 (blue) and W_5 (red) and the depth temperatures measured in situ, versus the theoretical value A_{Theo} of the
444 solar parameter computed (see Appendix C) using the parameterization of Bréon and Henriot (2006). The black
445 line represents the values of ΔT computed (see text), for the conditions of each observation, following Fairall et
446 al. (1996), Wick et al. (2005) and Zeng and Beljaars (2005). Right y axis: Number of IASI-drifter collocations
447 used, denoted by grey boxes in the figure. Lower panel: The RSDs associated with the above described results.

448
449 Some atmospheric situations may affect the quality of the restitutions through two main effects.
450 Firstly, the presence of unscreened clouds tends to reduce the radiance observed by the satellite, and
451 the retrieved SST is then underestimated. Although they are relatively rare, such cases exist in our
452 collocations, as indicated by the slight shift toward negative values of the mean of the
453 $\Delta T_{\text{IASI}} = T_{\text{IASI}} - T_{\text{Depth}}$ distribution when compared to the median (see Table 1). In the 3.6-4.0 μm
454 range, the presence of aerosols may also contaminate the restitutions, the main contributors being the
455 mineral dusts and, to a lesser extent, the sea-salt coarse-mode which are usually confined inside the
456 bottom part of the boundary layer to which infrared sounders are weakly sensitive (see e.g. Pierangelo
457 et al., 2013). These aerosols may make two opposite contributions. Firstly, they reduce the radiance
458 collected by the satellite by absorbing the radiation, leading to an underestimation of both the retrieved
459 SST and A_{Fit} parameter. This effect is however relatively small in the mid-infrared region used here,
460 and corresponds to an error smaller than 0.5 K (see e.g. sensitivity studies in Peyridieu et al., 2013),
461 especially after filtering every observations with a DAOD retrieved at 10 μm lower than 0.2, as it is
462 explained in Sec. 3.1. Secondly, in the 3.6-4.0 μm spectral range, aerosols may also act on the
463 observed radiance by scattering the radiation, principally that coming from the sun. This increases the
464 solar contribution to the measured spectra, leading to an overestimation of both the SST and A_{Fit} , with
465 and impact all the more important when the collected solar flux is large. For the majority of the
466 observations analyzed here, for which $A_{\text{Theo}} < 0.5$, this effect is negligible (as for nighttime conditions).
467 In contrast, for extreme cases with $A_{\text{Theo}} > 3$, the scattering of solar light by aerosols can lead to errors
468 on the retrieved SST of up to 3-4 kelvin and to an overestimation on A_{Fit} reaching 50%, according to

469 synthetic simulations (no shown) carried out for a DAOD=0.2. When analyzing the results obtained,
470 and in particular those in Figs. 4 and 5, we conclude that such extreme cases are not so frequent in the
471 collocations retained for this study. Indeed, in Fig. 4, no significant deviation from the linear fit is
472 observed when A_{Theo} increases, and Fig. 5 does not indicate any large overestimation of the SST for
473 $A_{\text{Theo}} > 3$ when compared to the results obtained for smaller A_{Theo} values. These positive findings can be
474 explained by the fact that the potentially large contributions of scattered solar light are due to the
475 presence of transported mineral dust, a phenomenon which principally occurs during the summer over
476 the Atlantic, within the "dust belt" between 0° and 30°N (Peyridieu et al., 2013), whereas the "glint
477 situations" with large A_{Fit} values are located at higher latitude during this season (see e.g. Fig. 3).
478 Some errors may appear in the spring where the "glint" observations are located close to the equator
479 and some local overestimations of the SST are thus expected where dusts are then principally located
480 [see again (Peyridieu et al., 2013)]: In the Guinean Gulf, within the "dust belt" over the Atlantic from
481 the South-West of Africa to the North of Brazilian coasts, and close to coasts in the Indian ocean. Their
482 impact in these regions is however likely quite limited, given the small AOD and the low-altitude
483 transport involved (Peyridieu et al., 2013 ; Yu et al., 2019). These statements are confirmed by the
484 fact that the bias and the standard deviation in our restitutions remain practically unchanged when a
485 more strict filtering of dusty scenes [DAOD<0.03, as it was done for nighttime observations in Capelle
486 et al. (2022)] is applied. For $A_{\text{Theo}} > 1$, the ΔT_5 difference remains unchanged while the standard
487 deviation reduces from 0.38 to 0.36 K. In conclusion, if scenes containing aerosols are not frequent in
488 the retained observations, aerosols may contribute to noise in our SST retrievals, but this effect is
489 limited by the filtering applied on the DAOD. Finally, the quality of the results can be affected by
490 errors on the input data used, such as those on the water vapor and temperature profiles, on the sea-
491 surface emissivity, in particular for strong winds, and on the spectroscopy (i.e. water vapor
492 continuum). Their impacts are however limited, as demonstrated by the sensitivity study in the
493 Appendix of Capelle et al. (2022).

494

495

496 **5. Conclusion and perspectives**

497 We have shown that, even when solar light largely contributes to IASI radiances, the latter can
498 be used for accurate sea-surface temperature (SST) retrievals, provided that a suitable physically-
499 based radiative-transfer model is used. This is achieved, thanks to the availability of many mid-
500 infrared channels, by fitting a wave-slope-probability dependent parameter which turns out to be in
501 good agreement with direct theoretical predictions. The SSTs retrieved from numerous spectral
502 channels in two windows centered near 3.7 and 4.0 μm are then very consistent and in excellent
503 agreement with in-situ depth-temperature measurements after correction of the depth-to-skin
504 difference. Indeed, the associated median biases are below 0.05 K with robust standard deviations
505 lower than 0.35 K regardless of the solar contribution, even when the latter increases the observed
506 brightness temperature by several tens of kelvin.

507 These results open renewed perspectives for the treatment of mid-infrared daytime radiances
508 collected by hyperspectral sounders such as IASI, which are beyond the scope of this methodology
509 paper but deserve investigation in the future. This is obviously the case for SST retrievals and the
510 study of the diurnal cycle for which the radiances provided by IASI at 9:30 AM and 9:30 PM (local
511 time at the Equator) could be complemented by those collected at other local times by hyperspectral
512 sounders such as AIRS (Ruzmaikin et al., 2017), CrIS (Aumann et al., 2021), and potential future
513 geostationary instruments. From this point of view, long time series may contribute to the still open
514 issue (Ruzmaikin et al., 2017) of the Diurnal Temperature Range over seas. Perspectives are also
515 opened, among others, for the exploitation of the information contained in the high frequency lines of
516 the 4.3 μm CO_2 band [which are sensitive to both the temperature (Susskind et al., 2003 and 2010) and
517 the CO_2 amount (Crevoisier et al., 2003) in the bottom part of the atmosphere], and the determination
518 of atmospheric amounts of species, such as HDO (Herbin et al., 2009), showing signatures at high
519 frequencies in IASI recordings. More generally, the optimal use of the mid-infrared region is among
520 the priorities for future infrared sounders such as IASI-NG (Crevoisier et al., 2014).

521

522 **Declaration of Competing Interest**

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

525

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532

533

534

Appendices

535 Although some of the equations given below can be found in (or derived from) previously published
536 papers (Masuda et al., 1988 ; Chen et al., 2013 ; Br on, 1993 ; Br on and Henriot, 2006 ; Cox and
537 Munk, 1954), we reproduce them here in order to provide self-sufficient information to the reader.

538

539 **Appendix A: The bidirectional reflectivity ρ**

540 Since the (infrared) wavelengths used in this study are much smaller than all the spatial scales
541 associated with the geometry of the sea surface, the reflection of solar radiation on the ocean is driven
542 by the laws of geometrical optics. It is thus specular, and collecting along the $\vec{u}(\theta_I, \varphi_I)$ observation
543 direction photons emitted by the sun along the $-\vec{u}(\theta_S, \varphi_S)$ vector (see Fig. 1) requires an ad hoc wave
544 slope. The latter must have a normal vector $\vec{u}_\perp(\theta_I, \varphi_I, \theta_S, \varphi_S)$ along the direction defined by
545 $\vec{u}(\theta_I, \varphi_I) + \vec{u}(\theta_S, \varphi_S)$. This unitary vector is, in the axis frame of Fig. 1, defined by the coordinates:

$$546 \quad \vec{u}_\perp(\theta_I, \varphi_I, \theta_S, \varphi_S) = \left(\begin{array}{c} \sin(\theta_I)\cos(\varphi_I) + \sin(\theta_S)\cos(\varphi_S) \\ \sin(\theta_I)\sin(\varphi_I) + \sin(\theta_S)\sin(\varphi_S) \\ \cos(\theta_I) + \cos(\theta_S) \end{array} \right) / N, \quad (\text{A1})$$

547 where $N = \sqrt{2 + 2 \sin(\theta_I) \sin(\theta_S) \cos(\varphi_S - \varphi_I) + 2 \cos(\theta_S) \cos(\theta_I)}$. The angle of incidence
 548 $\theta_{\text{Inc}}(\theta_I, \varphi_I, \theta_S, \varphi_S)$ on the surface defined by this normal vector is such that:

$$549 \quad \cos[\theta_{\text{Inc}}(\theta_I, \varphi_I, \theta_S, \varphi_S)] = \sqrt{\frac{1 + \sin(\theta_I) \sin(\theta_S) \cos(\varphi_S - \varphi_I) + \cos(\theta_S) \cos(\theta_I)}{2}}. \quad (\text{A2})$$

550 The bidirectional reflectivity $\rho(\sigma, \theta_I, \varphi_I, \theta_S, \varphi_S) = \rho(\sigma, \theta_{\text{Inc}})$ can then be obtained using Fresnel's
 551 coefficients, Snell's law of refraction and the complex refractive index of sea water $n_{\text{SW}}(\sigma)$ as:

$$552 \quad \rho(\sigma, \theta_{\text{Inc}}) = [R_{//}^2(\theta_{\text{Inc}}) + R_{\perp}^2(\theta_{\text{Inc}})]/2, \quad (\text{A3})$$

553 with

$$554 \quad R_{//}(\theta_{\text{Inc}}) = -\frac{n_{\text{SW}}(\sigma) \cos(\theta_{\text{Inc}}) - \cos[\theta_{\text{Trans}}(\theta_{\text{Inc}}, \sigma)]}{n_{\text{SW}}(\sigma) \cos(\theta_{\text{Inc}}) + \cos[\theta_{\text{Trans}}(\theta_{\text{Inc}}, \sigma)]}, \quad (\text{A4})$$

$$R_{\perp}(\theta_{\text{Inc}}) = +\frac{\cos(\theta_{\text{Inc}}) - n_{\text{SW}}(\sigma) \cos[\theta_{\text{Trans}}(\theta_{\text{Inc}}, \sigma)]}{\cos(\theta_{\text{Inc}}) + n_{\text{SW}}(\sigma) \cos[\theta_{\text{Trans}}(\theta_{\text{Inc}}, \sigma)]}$$

555 in which the spectrally-dependent angle $\theta_{\text{Trans}}(\theta_{\text{Inc}}, \sigma)$ of the transmitted radiation is such that:

$$556 \quad \sin[\theta_{\text{Trans}}(\theta_{\text{Inc}}, \sigma)] = \sin(\theta_{\text{Inc}}) / n_{\text{SW}}(\sigma). \quad (\text{A5})$$

557 Note that, in the preceding equations, the index of refraction of air was (safely) replaced by unity.

558

559 **Appendix B: Sensitivity of the retrieved SSTs to the input parameters**

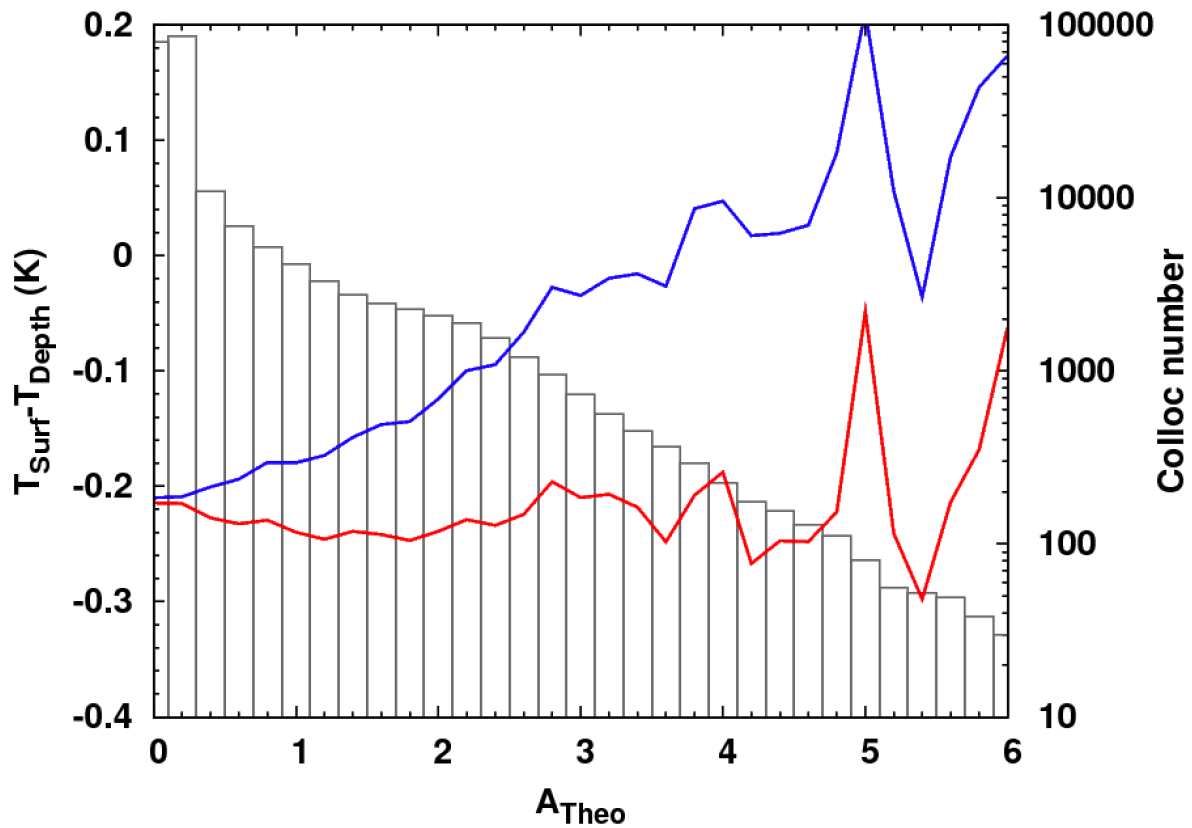
560 In Capelle et al. (2022), the sensitivity of SSTs retrieved in different windows of IASI spectra to
 561 various input parameters was studied. This included the influence of errors on the water vapor
 562 continuum parameterization, on the atmospheric water and temperature vertical profiles, and on the
 563 sea-surface emissivity. This analysis is thus not made here and the reader interested by this topic is
 564 invited to consult the appendices of Capelle et al. (2022). This previous analysis must here be
 565 complemented, since the treatment of daytime IASI spectra presented in this paper involves two new
 566 inputs: The solar spectrum and the bidirectional reflectivity (calculated from the index of refraction of
 567 water as described above).

568 It is obvious that any wavelength-independent scaling-factor error on the solar spectrum and/or
 569 reflectivity has no influence on the retrieved SSTs since it is automatically corrected through the
 570 adjustment of the solar parameter A (see Sec. 3.2 of the main text). In contrast, if the variations of the

571 relative error with σ within the spectral range used for the retrievals are wrong, this will impact the
572 retrieved SST. In order to quantify this effect, we have reanalyzed all IASI spectra after applying a
573 multiplicative factor $f(\sigma) = 1 + 0.01(\sigma - \bar{\sigma})/\Delta\sigma$ to the solar spectrum $I_{\text{Sun}}^0(\sigma)$ in Eq. (8) of the main
574 text [which is strictly equivalent to changing the bidirectional reflectivity $\rho(\sigma, \theta_I, \varphi_I, \theta_S, \varphi_S)$ by the
575 same factor], where $\bar{\sigma} = 2620 \text{ cm}^{-1}$ and $\Delta\sigma = 280 \text{ cm}^{-1}$. This leaves the solar spectrum unchanged at
576 the center of the range covered by windows W_4 and W_5 and changes it by +0.5 % (resp. -0.5 %) at the
577 point of highest (resp. lowest) frequency.

578 Figure A1 displays the evolutions of the medians ΔT s retrieved in window W_5 using the original
579 (Planck function at 5657 K) and modified [after applying the multiplicative factor $f(\sigma)$] solar spectra
580 versus the solar parameter A_{Theo} . The difference observed between the two resulting ΔT s is
581 proportional to A_{Theo} , with a coefficient of about 0.05. This shows that a perturbation of 1 % of the
582 spectral dependence of either $I_{\text{Sun}}^0(\sigma)$ or $\rho(\sigma, \theta_I, \varphi_I, \theta_S, \varphi_S)$ leads to a SST change of about 0.3 K for
583 a large solar contribution corresponding to $A_{\text{theo}}=6$. This significant sensitivity of our results to such a
584 perturbation implies that a careful choice of both $I_{\text{Sun}}^0(\sigma)$ and $\rho(\sigma, \theta_I, \varphi_I, \theta_S, \varphi_S)$ must be made. From
585 the literature, a large number of solar spectra are available [see references in Platnick et al. (2008) and
586 in Coddington et al. (2019)]. Analysis of several of them shows that they involve spectral dependences
587 differing from 1 to 3% when compared to the Planck function used here. The variability of the spectral
588 dependence of $\rho(\sigma, \theta_I, \varphi_I, \theta_S, \varphi_S)$, linked to the uncertainties on the refractive index of sea water in
589 the 3.6-4.0 μm region, seems to be less important. Indeed, comparing reflectivities computed from the
590 data of Hale and Querry (1973) and of Downing and Williams (1975), for example, shows that the
591 variation of the spectral dependence of $\rho(\sigma, \theta_I, \varphi_I, \theta_S, \varphi_S)$ is of about 0.3%. As shown by Fig. A1, any
592 error on the spectral dependence of $I_{\text{Sun}}^0(\sigma)$ and/or $\rho(\sigma, \theta_I, \varphi_I, \theta_S, \varphi_S)$ will cause, through their
593 participations in Eq. (8), an artificial and wrong variation of the retrieved $\Delta T = T_{\text{Skin}} - T_{\text{Dept}}$ with A_{Theo} . It
594 turns out that the choices we made, of a Planck function at $T=5657 \text{ K}$ for the sun radiance together
595 with the refractive index of sea water from Downing and Williams (1975), lead to a pair with which
596 the retrieved SSTs are, as they should be, practically independent of the solar contribution (i.e. of

597 A_{Theo}). Finally note that the black body temperature of 5657 K retained for the sun is that obtained, for
 598 the central wavelength (3.82 μm) of the interval used in this paper, using Eq. (6) of Platnick and
 599 Fontenla (2008) and that it leads to solar radiances within the uncertainties on the solar spectrum
 600 [which are discussed in Platnick and Fontenla (2008) and can be estimated from Fig. 1 of the same
 601 article].
 602
 603



604
 605 **Figure A1:** Left y axis: As in Figure 5 of the main text, average (over all observations using a bin of
 606 $\Delta A_{\text{Theo}}=0.2$) differences $\Delta T_5 = \bar{T}_5 - T_{\text{Depth}}$ between the sea-surface skin temperatures retrieved from
 607 IASI spectra in window W_5 and the depth temperatures measured in situ, for the solar spectrum used
 608 in this study (Planck function at $T=5657$ K), in red, and after multiplying this function by a factor
 609 $f(\sigma) = 1 + 0.01(\sigma - \bar{\sigma}) / \Delta\sigma$ (see text), in blue, versus the theoretical value A_{Theo} of the solar parameter
 610 computed (see Appendix C) using the parameterization of Bréon and Henriot (2006). The black line
 611 represents the values of ΔT computed for the conditions of each observation, following Fairall et al.

612 (1996), Wick et al. (2005) and Zeng and Beljaars (2005). Right y axis: Number of IASI-drifter
 613 collocations used denoted by grey boxes in the figure.

614

615 **Appendix C: The solar parameter A**

616 As explained in Appendix A, a reflecting wave with an ad hoc slope is needed for IASI to
 617 collect photons coming from the sun, characterized by the vector $\vec{u}_\perp(\theta_I, \varphi_I, \theta_S, \varphi_S)$ [see Eq. (A1)]
 618 orthogonal to its locally flat surface. The orientation of this surface is defined, in the axis frame of Fig.
 619 1, by the slopes:

$$\begin{aligned}
 \frac{\partial z}{\partial x} &= -\frac{\sin(\theta_S)\cos(\varphi_S) + \sin(\theta_I)\cos(\varphi_I)}{\cos(\theta_S) + \cos(\theta_I)} \\
 \frac{\partial z}{\partial y} &= -\frac{\sin(\theta_S)\sin(\varphi_S) + \sin(\theta_I)\sin(\varphi_I)}{\cos(\theta_S) + \cos(\theta_I)}
 \end{aligned}
 \tag{A6}$$

621 The probability $P(\partial z / \partial x, \partial z / \partial y)$ of waves to have these slopes was first investigated by Cox and
 622 Munk (1954) with results confirmed later on by Bréon and Henriot (2006). Provided that the \vec{x} axis is
 623 chosen along the up-wind direction, both studies propose to parameterize this probability through:

$$\begin{aligned}
 P(\partial z / \partial x, \partial z / \partial y) &= \frac{1}{2\pi\sigma_{//}\sigma_\perp} \exp\left[-\frac{\eta_{//}^2 + \eta_\perp^2}{2}\right] \times \left[1 - c_{21}(\eta_\perp^2 - 1)\eta_{//} / 2 - c_{03}(\eta_{//}^3 - 3\eta_{//}) / 6\right. \\
 &\quad \left. + c_{40}(\eta_\perp^4 - 6\eta_\perp^2 + 3) / 24 + c_{04}(\eta_{//}^4 - 6\eta_{//}^2 + 3) / 24 + c_{22}(\eta_{//}^2 - 1)(\eta_\perp^2 - 1) / 4\right].
 \end{aligned}
 \tag{A7}$$

624 with $\eta_{//} \equiv \frac{\partial z / \partial x}{\sigma_{//}}$ and $\eta_\perp \equiv \frac{\partial z / \partial y}{\sigma_\perp}$

625 Values of $\sigma_{//}$, σ_\perp , c_{21} , c_{03} , c_{40} , c_{04} , and c_{22} have been given by Cox and Munk (1954) and by
 626 Bréon and Henriot (2006), who parameterized them as a function of the wind speed at 12.5 m above
 627 the sea surface. Note that since Eq. (A6) is obtained in the axis frame of Fig. 1, Eq. (A7) can only be
 628 used after applying a change of $-\Delta\varphi$ to both φ_I and φ_S , where $\Delta\varphi$ is the angle between the (North-
 629 South) \vec{x} axis of Fig. 1 and the up-wind direction. Also recall that the angle $\theta_W(\theta_I, \varphi_I, \theta_S, \varphi_S)$
 630 defining the wave tilt with respect to the horizontal is given by:

$$\text{tg}(\theta_W)^2 = (\partial z / \partial x)^2 + (\partial z / \partial y)^2 = \frac{\sin^2(\theta_S) + \sin^2(\theta_I) + 2\sin(\theta_S)\sin(\theta_I)\cos(\varphi_S - \varphi_I)}{[\cos(\theta_S) + \cos(\theta_I)]^2}.
 \tag{A8}$$

632 In order to go further and obtain the expression of $A(\theta_I, \varphi_I, \theta_S, \varphi_S)$, one must take into account the
633 finite field of view of the IASI instrument and the wave-slope variations $\Delta(\partial z / \partial x)$ and $\Delta(\partial z / \partial y)$
634 associated with the solid angle within which radiation is collected. By using Eq. (A6) and changing
635 variables using the Jacobian matrix of the derivatives of $\partial z / \partial x$ and $\partial z / \partial y$ with respect to θ_I and φ_I ,
636 one obtains (e.g.: Chen et al., 2013), after some (tedious) algebra and the removal of the IASI-viewing
637 solid angle:

$$638 \quad A_{\text{Theo}}(\theta_I, \varphi_I, \theta_S, \varphi_S) = \frac{P(\theta_I, \varphi_I, \theta_S, \varphi_S)}{4 \cos(\theta_S) \cos^4(\theta_W)}, \quad (\text{A9})$$

639 where θ_W is given by Eq. (A8).

640 For calculations of A_{Theo} using the above given equations, one must know the wind direction and
641 speed at the (mast height) altitude of 12.5 m. Since we use data provided by the European Centre for
642 Medium-Range Weather Forecasts' (ECMWF) 5th Re-Analysis (ERA5) dataset (Hersbach and Dee,
643 2016) at the altitude of 10 m, a correction was made using the log law, i.e. (Stull, 1988):

$$644 \quad U(z) = \frac{U_*}{\kappa} \ln(z/z_0), \quad (\text{A10})$$

645 where κ ($=0.4$) is the von Karmann constant, U_* is the friction velocity, and z_0 is the surface
646 roughness length. The values of these last two parameters are obtained from knowledge of the wind
647 speed $U(z_r)$ at a reference height z_r (here 10 m) by iteratively solving Eq. (A10) with $z=z_r$ using the
648 relations (Smith, 1988):

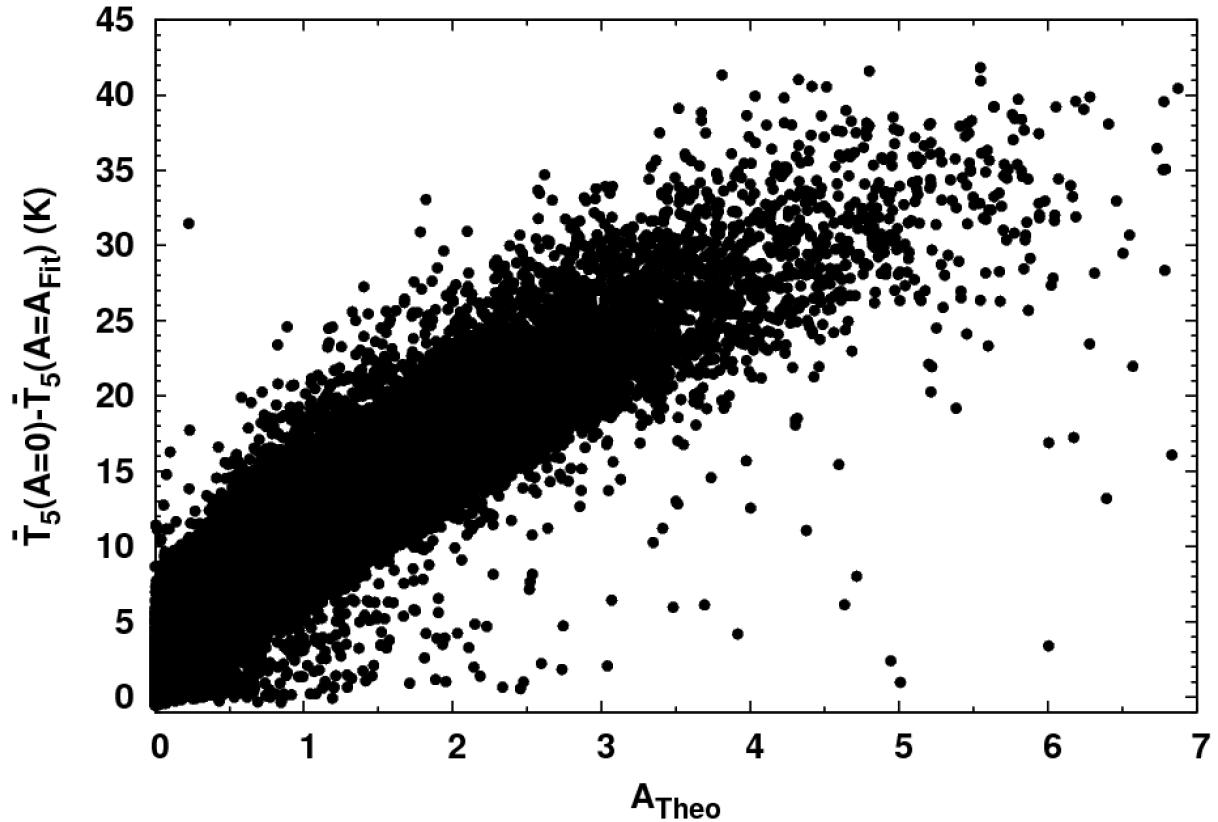
$$649 \quad U_* = \frac{\kappa U(z_r)}{\ln(z_r/z_0)}, \quad z_0 = \frac{0.11\nu}{U_*} + C \frac{U_*^2}{g}, \quad (\text{A11})$$

650 where ν ($=0.14 \text{ cm}^2/\text{s}$) is the dynamic viscosity of air, g ($=9.81 \text{ m/s}^2$) is the acceleration of gravity,
651 and C ($=0.018$) is Charnook's constant. Note that, for the wind speeds at 10 m associated with the IASI
652 observations treated in this study, which are all smaller than 20 m/s, the correction to 12.5 m is
653 relatively small (less than +2.6 %).

654

655 **Appendix D: The solar contribution**

656 When very unlikely steep wave slopes are involved (e.g. when IASI looks in a direction
 657 opposite to that of the sun), the solar contribution to the collected radiances is small (see Fig. 3 of the
 658 main text). Such observations, which are close to nighttime conditions from the radiative point of
 659 view, are of little interest for the validation of the methodology proposed in this paper. In order to
 660 easily detect them, and more generally to quantify the solar contribution for the analysis of the results
 661 presented in Sec. 4.2, we have considered the difference $\bar{T}_5(A=0) - \bar{T}_5(A=A_{\text{Fit}})$, between the
 662 average SST values retrieved in window W_5 , without and with the solar contribution taken into
 663 account. The results, displayed in Fig. A2 below as a function of the theoretical value of A for each
 664 observation, demonstrate (as could be expected) a strong correlation, the mean value of
 665 $\bar{T}_5(A=0) - \bar{T}_5(A=A_{\text{Fit}})$ for each A_{Theo} being well approximated, for $A_{\text{Theo}} > 0.5$ by
 666 $\bar{T}_5(A=0) - \bar{T}_5(A=A_{\text{Fit}}) \approx 10 + 6(A_{\text{Theo}} - 0.5)$ K. Finally note that, $\bar{T}_5(A=0)$ and $\bar{T}_5(A=A_{\text{Fit}})$ being
 667 averages over all spectral points in W_5 [see Eq. (9)], the values displayed in Fig. A2 can be
 668 significantly smaller than the difference $T(A=0, \sigma = \sigma_{\text{Max}}) - T(A=A_{\text{Fit}}, \sigma = \sigma_{\text{Max}})$ obtained from
 669 the highest frequency ($\sigma_{\text{Max}} = 2760 \text{ cm}^{-1}$) of the IASI spectrum (see, Fig. 2 of the main text). It is here
 670 worth mentioning that an error of + 30 K on the SST retrieved, disregarding the solar contribution,
 671 from the IASI radiance at the highest wavenumber (2760 cm^{-1}), implies that the sun here participates
 672 for about 75% of the recorded signal !
 673



674

675 **Figure A2:** Differences, $\bar{T}_5(A=0) - \bar{T}_5(A=A_{\text{Fit}})$, between the averaged SST values retrieved in window
 676 W_5 , without and with the solar contribution taken into account versus the theoretical value A_{Theo} of the solar
 677 parameter computed using the parameterization of Bréon and Henriot (2006).

678

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