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 sea surface temperature from the Chinese Gaofen-5 data

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Development of a split-window algorithm for estimating sea surface temperature from the Chinese Gaofen-5 data

Abstract: Sea surface temperature (SST) is an essential climate 30 variable that can be used to assess climate change. One kind of method 31 32 commonly used to estimate SST based on remote sensing measurements is the split-window (SW) algorithm. However, the derivation of the 33 34 linear SW algorithm does not appear to reflect reality because some 35 assumptions and approximations were used. Moreover, the quadratic SW equation cannot be interpreted theoretically although it maintains 36 37 the structure of the linear SW equation. The Gaofen-5 (GF-5) satellite 38 launch is planned for 2017. Focusing on exploring the mechanism of 39 the SW algorithm using GF-5 data, this study investigated the 40 assumptions and approximations used to derive the linear SW technique. Two revised equations of these assumptions and approximations were 41 42 developed. Combining the revised equations, a nonlinear SW algorithm was obtained that could be simplified to the quadratic equation. 43 44 Compared with previous research, this study focuses more on the 45 theoretical interpretation and improves our understanding of the semiempirical quadratic SW equation. The matchup dataset produced by the 46 47 European Organization for the Exploitation of Meteorological Satellites (EUMETSAT) Ocean and Sea Ice Satellite Application Facility (OSI-48 49 SAF) was used to validate the quadratic SW algorithm. A bias of -0.05 K and a RMSE of 0.53 K were obtained. 50

51 Keywords: Sea surface temperature; Split-window; Revision; GF-5; 52 Thermal infrared

53 **1. Introduction**

54 As an important parameter in the exchange of energy between the ocean and 55 the atmosphere, the sea surface temperature (SST) reflects both oceanic and

atmospheric variability on multiple temporal and spatial scales (Fisher 1958; 56 Liu and Minnett 2015). High-quality SST datasets are needed for many 57 applications, such as numerical weather prediction, ocean forecasting, and 58 59 climate change assessment (Pinardi et al. 2003; Barnett et al. 1993; Chelton and Wentz 2005; Donlon et al. 2007). Knowledge of the distribution of SST is also 60 useful for locating various species of fish (Simpson 1994). Such investigations 61 can be satisfied using satellite remote sensing data. However, accurate 62 determination of SST from satellite data is a difficult task because the at-sensor 63 measured radiances include the atmospheric absorption and emission (Liu et al. 64 2013). Thus, removal of the atmospheric effects is a key step in the accurate 65 retrieval of SST from remotely sensed data. 66

Despite the problem of atmospheric effects, retrieval of SST 67 information from space using thermal infrared (TIR) data began in 1970. 68 Anding and Kauth (1970) first demonstrated that the atmospheric effects can 69 70 be almost compensated for by simultaneously using the radiometric measurements in two properly selected TIR bands. Prabhakara et al. (1974) first 71 72 suggested the general method of estimating SST from two TIR channel 73 measurements. Therefore, the split-window (SW) technique for estimating SST was derived based on the previous works, with the general idea that the 74 atmospheric effects are proportional to the difference between the at-sensor 75 radiances measured simultaneously in two TIR channels (McMillin 1975; 76 Ulivieri et al. 1994; Coll and Caselles 1997; Rozenstein et al. 2014). For 77

78 nighttime retrieval, the channel near 3.7 µm is often used to improve the 79 accuracy of SST retrieval because it's a more transparent band, compared with the bands centered at 11 and 12 μ m (Barton 1983). However, there is significant 80 81 solar radiation at this wavelength that restricts the channel to be used for daytime SST retrieval (McClain, Pichel, and Walton 1985; Petrenko et al. 2014). 82 Since then, a variety of methods based on the SW technique have been 83 developed and improved to retrieve SST and LST (land surface temperature) 84 (McClain, Pichel, and Walton 1985; Becker and Li 1990; Sobrino, Li, and Stoll 85 1993; Niclòs et al. 2007; Qian et al. 2016). 86

In the derivation of the SW technique, some assumptions and 87 approximations were made to obtain the SST. One assumption is the first-order 88 89 Taylor approximation of the Planck function (Prabhakara, Dalu, and Kunde 1974; Becker 1987). Another assumption is that the atmospheric equivalent 90 temperatures in the two adjacent TIR channels were the same $(T_{ai} = T_{aj})$ 91 92 (McMillin 1975; Sobrino, Coll, and Caselles 1991). Notably, there are certain restrictions for these assumptions. As demonstrated in the literature (Sobrino, 93 Coll, and Caselles 1991; Becker 1987), the linear approximation of the Planck 94 function is generally accurate under the condition that T and T_i are close to each 95 other (T represents the atmospheric equivalent temperature or surface 96 97 temperature and T_i is the brightness temperature measured by the satellite). However, it is difficult to meet this condition due to the strong variability of 98 global atmospheric conditions. In addition, the hypothesis $T_{ai} = T_{aj}$ does not 99

appear to reflect reality. Therefore, these assumptions and approximations mustbe re-examined.

The Gaofen-5 (GF-5) satellite is expected to be launched in 2017. An 102 103 advantage of the multiple spectral-imager (MSI) onboard GF-5 satellite is the 104 high spatial resolution (40 meters for TIR channels). As a result, applications of the TIR data from GF-5 are different from those of other sensors with coarser 105 106 spatial resolutions. For example, the high resolution SST data of GF-5 can be used to monitor the thermal pollution produced by the nuclear power. Thus, 107 there is an urgent need to develop an algorithm that is suitable for retrieving 108 109 SST from GF-5/TIR data. In this paper, the investigation of the following assumptions and approximations: 1) the linearization of the Planck function and 110 111 2) the atmospheric equivalent temperatures in two TIR channels, which were assumed to be the same was undertaken based on the Chinese GF-5 data. We 112 aim to explore the mechanism of the SW algorithm further through revising 113 114 these assumptions and approximations. The paper is organized as follows: Section 2 describes the data used in this study. The theoretical revision and 115 derivation of the SW technique, including revision of the linearization of the 116 Planck function, revision of the $T_{ai} = T_{aj}$ hypothesis and analysis of the 117 developed SW algorithm, are documented in Section 3. The effect of instrument 118 noise on SST retrieval and the algorithm validation are described in Section 4. 119 The discussion is given in Section 5. Finally, Section 6 presents the conclusions. 120

121 **2. Data**

122 2.1 Chinese GF-5 data

With the launch of the China High-resolution Earth Observation System 123 (CHEOS), China has entered a new era of high resolution operations. GF-5 is 124 the fifth satellite in a series of CHEOS, scheduled to be launched in 2017. One 125 126 of the major sensors onboard the GF-5 satellite is the multiple spectral-imager (MSI) that includes 13 channels covering the spectral range from visible to TIR 127 and observes the earth almost at nadir. The channels centered at 10.8 µm and 128 11.95 μ m are two TIR channels (labeled CH_{10.8} and CH_{11.95}, respectively, 129 hereafter) suitable for SW method, with a spatial resolution of 40 meters. The 130 spectral response functions of CH_{10.8} and CH_{11.95} are shown in Figure 1. 131

132 2.2 Matchup data set

To assess the performance of the developed algorithm, Matchup dataset (MDS) 133 produced by the European Organization for the Exploitation of Meteorological 134 Satellites (EUMETSAT) Ocean and Sea-Ice Satellite Application Facility 135 136 (OSI-SAF) was collected. MDS was provided in NetCDF format, containing the fields of latitude, longitude, viewing zenith angle (VZA), acquisition time, 137 138 AVHRR at-sensor brightness temperatures, in situ SSTs, etc. AVHRR 139 brightness temperatures are coincident in time and space with the in situ SSTs. 140 From Figure 1, which also displays the spectral response functions of AVHRR

SW channels, we can see that the spectral configuration of GF-5/MSI and 141 142 AVHRR SW channels is similar. Considering the lack of available GF-5 data at present, the "true" GF-5 brightness temperature can be got from the AVHRR 143 measurements based on the relationship built by the simulated data for the 144 purpose of algorithm validation. The in situ SSTs recorded by drifting buoys 145 146 were collected from the Global Telecommunication System (GTS) with an 147 AVHRR pixel. Figure 2 shows the location distribution of in situ SSTs, indicating the almost global coverage of in situ measurement. 148



Figure 1. Spectral response functions for Gaofen-5 and AVHRR split-windowchannels.



152

153 Figure 2. Distribution of in situ sea surface temperatures on the global ocean.

154 2.3 Atmospheric profile data

Several sets of real atmospheric profiles, such as the Thermodynamic Initial 155 Guess Retrieval (TIGR) database has been widely used for the development of 156 SST and LST retrieval algorithms (Scott and Ch édin 1981; Ch édin et al. 1985). 157 In this work, the TIGR database TIGR2002_v1.1 was used as input to the 158 159 radiative transfer simulation (see Section 2.4). Due to the large size of the TIGR2002 v1.1 and concentrations of water vapor content (WVC) less than 1 160 g/cm^2 , it is reasonable to select different atmospheric profiles according to well-161 distributed values of WVC. Figure 3 shows the 104 atmospheric profiles 162 selected, with the atmospheric temperature in the lowest layer (T_0) varying from 163 232.25 K to 303.41 K and the WVC from 0.09 g/cm² to 5.69 g/cm², which 164 constructed a robust database capable of representing global atmospheric 165 conditions with a moderate number of samples and a nearly uniform WVC 166

distribution. Eighty-one profiles (referred to as TIGR_81) were used for
developing the SST retrieval algorithm and twenty-three profiles (referred to as
TIGR 23) were used for validation.



170

Figure 3. Plot of the total water vapor content (WVC) as a function of
atmospheric temperature in the lowest layer (T₀) for selected atmospheres.
TIGR_81 was used for algorithm development (black points) and TIGR_23
(red points) for algorithm validation.

175 2.4 Generation of the simulated database

To obtain an appropriate simulated database for developing a SST retrieval algorithm for GF-5 TIR data, the atmospheric radiative transfer model MODTRAN (Berk et al. 1999) was used to simulate the spectral atmospheric parameters of spectral transmittance τ_{λ} , spectral atmospheric upwelling radiance $R_{atm_{\lambda}}^{\dagger}$ and spectral atmospheric downwelling $R_{atm_{\lambda}}^{\dagger}$. The channeleffective atmospheric parameters τ_i , $R_{atm_{\lambda}}^{\dagger}$ and $R_{atm_{\lambda}}^{\dagger}$ can be obtained by

182	integrating these spectral variables with spectral response functions in CH _{10.8}
183	and CH _{11.95} . The channel brightness temperature T_i at the top of the atmosphere
184	(TOA) can then be determined according to the radiative transfer equation
185	(RTE) (Coll and Caselles 1994; Niclòs et al. 2007) by inverting the Planck
186	function in combination with a wide range of SSTs, considering the VZA of 0 $^\circ\!\!.$
187	For a more realistic simulation, the SSTs reasonably vary with T ₀ . Specifically,
188	five SSTs ($T_0 - 5$ K, $T_0 - 2$ K, T_0 K, $T_0 + 2$ K and $T_0 + 5$ K) were considered in
189	this study. All of the data were obtained considering the emissivity to be equal
190	to one because the ocean surface radiates almost as a blackbody at infrared
191	wavelengths (McClain, Pichel, and Walton 1985). A flow chart of generation
192	of the simulated data is presented in Figure 4.



Figure 4. The procedure of generating the simulated data.

195 **3. Method of revising the linear SW algorithm**

193

194

The theoretical basis for the SST retrieval algorithm relies on the RTE. Assuming that: 1) the first-order Taylor approximation of the Planck function was used and 2) the atmospheric equivalent temperatures in two TIR channels were equal ($T_{ai} = T_{aj}$), a typical linear SW algorithm (Sobrino, Li, and Stoll 1993; McClain, Pichel, and Walton 1985; Barton 1995; Kilpatrick, Podestfi, and Evans 2001) can be obtained:

202
$$T_s = T_i + A(T_i - T_i)$$
 (1)

where T_s is the sea surface temperature (*i.e.*, SST; hereafter, SST is used 203 204 interchangeably with T_s), T_i and T_j are the brightness temperatures in channels *i* and *j* at the TOA, and *A* is the coefficient defined by $A = (1 - \tau_i) / (\tau_i - \tau_j)$ in 205 which τ_i and τ_j are the transmittances through the atmosphere from the surface 206 to the satellite in channels i and j. Eq. (1) indicates that a linear relationship 207 exists between $T_s - T_i$ and $T_i - T_j$. However, an empirical quadratic relationship 208 was found when relating $T_s - T_i$ to $T_i - T_j$. Coll et al. (1994) proposed a quadratic 209 SW equation but no physical interpretation. In the next section, we will 210 investigate the derivation of the quadratic SW equation by re-examining the 211 212 two assumptions and approximations mentioned above.

213 3.1 Revision of the linearization of the Planck function

Based on the RTE, Eq. (2) can be obtained by using Taylor's expansion of thePlanck function,

216
$$T_i = T_{ai} + \tau_i (T_s - T_{ai}) + \Delta T_i$$
(2)

where ΔT_i is the error in T_i caused by linearizing the Planck function. In the published literature, ΔT_i is small and always neglected (McClain, Pichel, and Walton 1985; Walton et al. 1998; Prabhakara, Dalu, and Kunde 1974). Using the simulated data, the calculated results of ΔT_i for CH_{10.8} and CH_{11.95} by Eq. (2) are shown in Figure 5 (a) and (b). It can be observed that a RMSE of 0.10
K and a bias of 0.07 K were obtained for CH_{10.8}, and those of CH_{11.95} were 0.11
K and 0.08 K, respectively. Writing Eq. (2) for two channels, one can obtain
Eq. (3),

225
$$T_{s} = T_{i} + A(T_{i} - T_{i}) + \Delta T_{s1} + \Delta T_{s2}$$
(3)

where $\Delta T_{s1} = -\Delta T_i - A(\Delta T_i - \Delta T_j)$ with the same *A* as in Eq. (1), $\Delta T_{s2} = A_a(T_{ai})$ 226 227 - T_{aj} with $A_a = -(1 - \tau_i)(1 - \tau_j) / (\tau_i - \tau_j)$. We can see that ΔT_{s1} is the error of T_s retrieval caused by linearizing the Planck function and ΔT_{s2} , which will be 228 presented in Section 3.2, is the influence of the hypothesis $T_{ai} = T_{aj}$ on T_s 229 retrieval. Figure 5 (c) displays the results of ΔT_{s1} , which is within the range of 230 -0.4~0.5 K. The negative bias (-0.06 K) of ΔT_{s1} indicates that the surface 231 temperature was overestimated due to the linearization of the Planck function, 232 with RMSE = 0.10 K. 233

234



Figure 5. The error caused by the linearization of the Planck function for channels with central wavelengths of (a) 10.8 μ m, (b) 11.95 μ m and (c) for SST. To revise the error caused by the linearization of the Planck function, the second-order derivative of Taylor's expansion was considered. Based on the RTE, ΔT_i in Eq. (2) can be rewritten as the following expression:

245
$$\Delta T_{i} = \frac{\frac{1}{2} (\frac{\partial^{2} B_{i}(T)}{\partial T^{2}})_{T_{i}} [(1 - \tau_{i})(T_{ai} - T_{i})^{2} + \tau_{i}(T_{s} - T_{i})^{2}]}{(\frac{\partial B_{i}(T)}{\partial T})_{T_{i}}}$$
(4)

where $\left(\frac{\partial B_i(T)}{\partial T}\right)_{T_i}$ and $\left(\frac{\partial^2 B_i(T)}{\partial T^2}\right)_{T_i}$ are the first-order and second-order derivatives of the Planck function at temperature T_i , respectively. Eq. (4) shows that ΔT_i is described by a complex expression. Parameterization of Eq. (4) is necessary. Considering the simplified case of Eq. (2) in which ΔT_i was regarded as zero, Eq. (2) can also be rewritten as:

251
$$(1-\tau_i)(T_i-T_{ai}) = \tau_i(T_s-T_i)$$
 (5)

Putting the square on both sides of Eq. (5), one can obtain Eq. (6) by simplemathematical manipulation,

254
$$(1-\tau_i)(T_i - T_{ai})^2 = \tau_i (T_s - T_i)^2 \frac{\tau_i}{1-\tau_i}$$
(6)

In addition, using the approximation of the Planck function in the work of Price(1984),

$$B_i(T_i) = a_i T_i^{n_i} \tag{7}$$

where a_i and n_i are constants in a given channel, Eq. (8) can be obtained:

259
$$\left(\frac{\partial^2 B_i(T)}{\partial T^2}\right)_{T_i} / \left(\frac{\partial B_i(T)}{\partial T}\right)_{T_i} = \frac{n_i - 1}{T_i}$$
(8)

260 Combining Eqs. (6) and (8), ΔT_i can be parameterized as $\frac{1}{2}(n_i - 1)\frac{(T_s - T_i)^2 \tau_i}{T_i(1 - \tau_i)}$.

261 As shown in Figure 6, there is a strong dependence between ΔT_i and

262
$$\frac{(T_s - T_i)^2 \tau_i}{T_i(1 - \tau_i)}$$
, with sufficient accuracy of T_i (RMSE lower than 0.01 K) for both

263 channels. Based on Figure 6, ΔT_i is rewritten as:

$$\Delta T_i = \alpha_i \frac{(T_s - T_i)^2 \tau_i}{T_i (1 - \tau_i)} \tag{9}$$

where α_i is the regression coefficient, which is 1.40 for CH_{10.8} and 1.21 for

266 CH11.95.



Figure 6. ΔT_i versus $(T_s - T_i)^2 \tau_i / (T_i (1 - \tau_i))$ for Gaofen-5 TIR channels centered at (a) 10.8 µm and (b) 11.95 µm. Here, T_s is the surface temperature, T_i is the simulated brightness temperature, τ_i is the transmittance and ΔT_i is the difference between the simulated and estimated brightness temperatures from Eq. (2).

274 **3.2** Revision of the $T_{ai} = T_{aj}$ hypothesis

If the hypothesis of $T_{ai} = T_{aj}$ is used for the T_s retrieval, ΔT_{s2} in Eq. (3) is 0. However, according to the calculated $T_{a10.8}$ and $T_{a11.95}$ using the thermal-path atmospheric upwelling radiance generated from the simulation, ΔT_{s2} ranges from about -6~2 K, as seen in Figure 7. It can be concluded that use of the T_{ai} $= T_{aj}$ hypothesis can lead to large error in T_s retrieval, with the RMSE of 1.74 K and bias of -0.88 K.



281

Figure 7. The error caused by the hypothesis of $T_{a10.8} = T_{a11.95}$ for SST retrieval. Here, $T_{a10.8}$ and $T_{a11.95}$ are the atmospheric equivalent temperatures in Gaofen-SW channels.

Notably, the discrepancy between T_{ai} and T_{aj} must be taken into account in SST retrieval from satellite observations (Franqois and Ott1 é 1996). From Figure 8, it can be observed that 1) there is a discrepancy between $T_{a10.8}$ and $T_{a11.95}$ for GF-5 data, with $T_{a11.95} > T_{a10.8}$ for low $T_{a10.8}$ and $T_{a11.95} < T_{a10.8}$ for high $T_{a10.8}$. The maximum difference between $T_{a10.8}$ and $T_{a11.95}$ is almost 4 K; 2) $T_{a11.95}$ and $T_{a10.8}$ are approximately equal only in a small range of atmospheric 291 conditions, at approximately $T_{a10.8}$ between 275-285 K; 3) there is a linear 292 dependence between $T_{a10.8}$ and $T_{a11.95}$,

293
$$T_{a11.95} = aT_{a10.8} + b \tag{10}$$

where a = 0.9172 and b = 23.00, with RMSE = 0.50 K. Using this linear relationship, the SST residual calculated by Eq. (3) is shown in Figure 9. Compared with the result caused by the hypothesis of $T_{ai} = T_{aj}$, the RMSE is changed to 0.62 K and the bias is changed to -0.10 K.



298

Figure 8. The relationship between atmospheric equivalent temperatures in two

300 Gaofen-5 TIR channels (labeled $T_{a10.8}$ and $T_{a11.95}$).



301

Figure 9. The SST residual obtained by Eq. (3) when the linear dependence ofthe atmospheric equivalent temperatures in two TIR channels was used.

Combining Eq. (9) and Eq. (10), the SST can be obtained by writing Eq.

305 (2) for two SW channels,

$$SST = MT_{10.8} + NT_{11.95}$$
(11)

307 where
$$M = \frac{A_4}{2(A_1 - A_2 \frac{T_{10.8}}{T_{11.95}})}$$
, $N = \frac{\sqrt{A_4^2 + 4(\frac{A_1}{T_{10.8}} - \frac{A_2}{T_{11.95}})(A_5 T_{10.8} + A_6 T_{11.95} + A_3)}}{2(A_1 \frac{T_{11.95}}{T_{10.8}} - A_2)}$

308 with

309
$$A_1 = \frac{a\alpha_{10.8}(1-\tau_{11.95})\tau_{10.8}}{1-\tau_{10.8}}, A_2 = \frac{\alpha_{11.95}(1-\tau_{10.8})\tau_{11.95}}{1-\tau_{11.95}}, A_3 = b(1-\tau_{10.8})(1-\tau_{11.95}),$$

$$\begin{array}{ll} \textbf{310} \qquad A_4 = 2(A_1 - A_2) - a(1 - \tau_{11.95})\tau_{10.8} + (1 - \tau_{10.8})\tau_{11.95} \quad , \quad A_5 = -A_1 + a(1 - \tau_{11.95}) \quad , \\ \textbf{311} \qquad A_6 = A_2 - (1 - \tau_{10.8}) \end{array}$$

312 3.3 Analysis of the nonlinear SW algorithm

Equation (11) is complex, requiring analysis and simplification. According to
the simulated data, *M* ranged from 0.9620~0.9941 and *N* from 0.0328~0.0394.
Taking the value of *M* approximately close to one, Eq. (11) can be rewritten as:

316
$$SST - T_{10.8} = (M - 1)(T_{10.8} - T_{11.95}) + (M - 1 + N)T_{11.95}$$
(12)

Since (M-1) is close to 0, the first term of Eq. (12) (*i.e.*, $(M-1)(T_{10.8}-T_{11.95})$) 317 is small even if multiplied by the maximum of $(T_{10.8} - T_{11.95})$ (approximately 4 318 K). In contrast to the small value of the first term, the second term (*i.e.*, (M-1)319 320 $(+ N)T_{11.95}$) makes the main contribution to Eq. (12) (see Figure 10), because of the large value of $T_{11.95}$. Taking the structure of the SW algorithm into 321 consideration, $(M - 1 + N)T_{11.95}$ should be the function of $(T_{10.8} - T_{11.95})$. 322 323 Therefore, the relationship between $(M - 1 + N)T_{11.95}$ and $(T_{10.8} - T_{11.95})$ was investigated further. As shown in Figure 11, $(M - 1 + N)T_{11.95}$ can be 324 parameterized using $(T_{10.8} - T_{11.95})$, with RMSE = 0.30 K. 325



Figure 10. Values of $(M - 1)(T_{10.8} - T_{11.95})$ and $(M - 1 + N)T_{11.95}$ in Eq. (12) versus the atmospheric water vapor content (WVC).



329

Figure 11. The relationship between $(M - 1 + N)T_{11.95}$ in Eq. (12) and the difference of the brightness temperatures in SW channels $(T_{10.8} - T_{11.95})$.

Based on the above analysis, Eq. (12) can be simplified as:

333
$$SST - T_{10.8} = A(T_{10.8} - T_{11.95})^2 + B(T_{10.8} - T_{11.95}) + C$$
(13)

where *A*, *B* and *C* are the coefficients. Using the least-square fitting method, the coefficients A = 0.4253, B = 1.123 and C = 0.28 were obtained using the simulated data, with RMSE = 0.30 K. Figure 12 shows the histogram of the difference between the actual SST and that obtained by Eq. (13).





Figure 12. Histogram of the differences between the actual and estimated SSTsusing Eq. (13).

341

342 **4. Error analysis and validation**

343 *4.1 Error of the instrument noise*

The accuracy of the estimated SST will essentially depend on the radiometric 344 345 performance of the instrument. The noise equivalent differential temperature (NE Δ T) in infrared channels is designed to be 0.2 K for GF-5 TIR data. To 346 evaluate the performance of the quadratic algorithm in this study, a simulation 347 of the effect of satellite noise was performed using a set of randomly generated 348 signal level perturbations with errors of 0.1 K, 0.2 K and 0.3 K for both channels. 349 350 The RMSEs between the true SSTs and those retrieved from the noise-added brightness temperatures are 0.49 K, 0.82 K and 1.20 K for NE $\Delta T = 0.1$ K, 0.2 351 K and 0.3 K, respectively, in both channels. 352

353 4.2 Validation with simulated data

To assess the general applicability of the quadratic SW equation to different atmospheric conditions, the accuracy of Eq. (13) was also evaluated using another set of data, TIGR_23. Figure 13 presents the error distribution between the true and the estimated SSTs, with RMSE = 0.3 K and bias = 0 K.



358

Figure 13. Histogram of the differences between the true and estimated SSTsbased on TIGR_23 data.

361 4.3 Validation using Matchup dataset

362 *4.3.1 Data processing*

The invalid values in MDS were first cleaned out. Considering that MSI instrument observes the earth almost at nadir, the data within the VZA of 20°, which contains 24231 pairs of in situ SSTs and AVHRR at-sensor brightness temperatures matchup data, was used in this study. In order to get the "true"

367	GF-5/MSI brightness temperatures, the relationship between GF-5/MSI and
368	AVHRR brightness temperatures was established using the simulated data for
369	each SW channel, as presented in Figure 14. It can be seen that there is a strong
370	linear relationship between GF-5/MSI and AVHRR brightness temperatures
371	with the RMSE no higher than 0.05 K for both channels. Using this relationship,
372	the "real" GF-5/MSI at-sensor brightness temperatures can be calculated from
373	AVHRR brightness temperatures in MDS. 24231 pairs of in situ SSTs and
374	coincident in time and space GF-5/MSI brightness temperatures were then
375	established. It should be noted that simulations may be significantly biased with
376	respected to observations due to modeling errors and not fully accuracy
377	atmospheric profiles. Observed data is also affected by uncertainties in
378	calibration, spectral response functions and residual cloud. Therefore, the
379	algorithm coefficients based on the observed data is needed to retrieve SST
380	from GF-5 satellite data. Among 24231 pairs of in situ SSTs and GF-5/MSI
381	brightness temperatures matchup data, 10000 pairs were used to obtain the
382	algorithm coefficients suitable for GF-5/MSI data, while the remaining 14231
383	pairs were used for validation purpose. According to the Figure 15, which
384	presents the quadratic relationship between buoy SSTs and GF-5/MSI
385	brightness temperatures, the coefficients $A = 0.1877$, $B = 1.845$ and $C = 1.07$ in
386	the quadratic SW algorithm were obtained for GF-5/MSI data, with the RMSE
387	= 0.52 K.



Figure 14. Plot of the simulated AVHRR and GF-5/MSI brightnesstemperatures for each of split-window channel.



391

Figure 15. Plot of (Buoy SST – $T_{10.8}$) and ($T_{10.8}$ - $T_{11.95}$). Here, Buoy SST is the sea surface temperature measured by drifting buoy, $T_{10.8}$ and $T_{11.95}$ are the GF-5/MSI brightness temperatures calculated from AVHRR brightness temperatures in MDS.

396 *4.3.2 Validation results*

Using the coefficients given in Section 4.3.1, SSTs were calculated from the
remaining GF-5/MSI data. Analyzing comparisons of GF-5/MSI SSTs with

buoy SSTs gives a bias of -0.05 K and a RMSE of 0.53 K, as shown in Figure 16. Among the 14231 pairs data, 95.45% of the differences between buoy SSTs and GF-5/MSI SSTs are within ± 1 K. From Figure 16, one may note that, there is a large error up to about 8 K. This may be related to the contribution of some materials floating on ocean or the incorrect measurement by accidental.



404

Figure 16. Buoy sea surface temperature minus sea surface temperatureobtained by GF-5/MSI.

407 **5. Discussion**

Although many studies report the quadratic SW algorithm, this study aims for a well understanding of the semi-empirical quadratic SW algorithm. The analyses were based on a comprehension of the derivation procedure of the linear SW equation. The SST errors resulted from the linearization of the Planck function were RMSE = 0.10 K and bias = -0.06 K, while the ones from the hypothesis of $T_{ai} = T_{aj}$ were 1.74 K and -0.88 K. Although the influence of the

linearization of the Planck function on SST retrieval was not obvious as the 414 effect of the $T_{ai} = T_{aj}$ hypothesis, in order to interpret the physical derivation of 415 the quadratic SW algorithm, the second-order derivative of Taylor's expansion 416 of the Planck function and the linear dependence between atmospheric 417 418 equivalent temperatures in two SW channels were considered. The obtained nonlinear SW algorithm by combining the two revisions of the Planck function 419 420 linearization and of the $T_{ai} = T_{aj}$ hypothesis is complex. However, it can be simplified to the quadratic structure of $(T_i - T_j)$, meaning that the nonlinear SW 421 algorithm is equivalent to the quadratic SW equation. Compared with the 422 423 previous studies, which presented the quadratic relationship between TOA brightness temperatures and the surface temperature by maintaining the 424 425 structure of linear SW algorithm but no physical interpretation, this study makes the physical interpretation of the semi-empirical quadratic SW algorithm 426 clear theoretically and improves our understanding of the quadratic SW 427 algorithm. 428

429 **6.** Conclusions

Some assumptions and approximations were used in the derivation of the linear
SW equation. Using the simulated data, this work carefully evaluated these
assumptions and approximations based on the RTE. We found that these
assumptions and approximations were not precise for SST retrieval. Therefore,
the revised equations for the Planck function linearization and for the

relationship between the atmospheric equivalent temperatures in SW channels
of GF-5 data were created. Based on these studies, a nonlinear SW algorithm
was obtained. Further analysis of the nonlinear SW algorithm clarified that it is
equivalent to the quadratic SW equation but highlights the theoretical
interpretation.

The effects of instrument noise on SST retrieval using the developed
quadratic SW algorithm were analyzed. The total errors were 0.49 K, 0.82 K
and 1.20 K for NEΔTs of 0.1 K, 0.2 K and 0.3 K, respectively. The validation
using the MDS produced by EUMETSAT OSI-SAF presented a RMSE of 0.53
K and a bias of -0.05 K.

A GF-5 satellite carrying a MSI instrument with narrow swaths and a 445 446 high resolution of 40 meters is scheduled to be launched in 2017. The analysis of GF-5 satellite data will be performed in future work when the data is 447 available. Because land surface is much more complicated than sea surface and 448 449 the LST differs significantly from the air temperature near the surface, large errors may be introduced by the assumptions and approximations used in the 450 derivation of the linear SW method. This hypothesis will be tested in future 451 452 work.

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