# 1 Retrieval of Solar-induced Chlorophyll Fluorescence from Satellite 2 Measurements: Comparison of SIF between TanSat and OCO-2

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17	Abstract. Solar-induced chlorophyll fluorescence (SIF) is emitted during photosynthesis in plant leaves. It constitutes a small	
18	additional offset to reflected radiance and can be observed by sensitive instruments with high signal-to-noise ratio and spectral	
19	resolution. The Chinese global carbon dioxide monitoring satellite (TanSat), acquires measurements of greenhouse gas column	
20	densities. The advanced technical characteristics of the grating spectrometer (ACGS) onboard TanSat enable SIF retrievals	// '
21	from observations in the O2-A band. In this study, one year of SIF data was retrieved from Orbiting Carbon Observatory-2	$\mathbb{N}$
22	(OCO-2) and TanSat measurements using the IAPCAS/SIF algorithm. A comparison between the IAPCAS/SIF results	$\bigvee$
23	retrieved from OCO-2 spectra and the official OCO-2 SIF product (OCO2_Level 2_Lite_SIF.8r) shows a strong linear	
24	relationship ( $R^2 > 0.85$ ) and suggests <u>good</u> reliability of the <u>IAPCAS/SIF</u> retrieval algorithm. <u>Comparing global distributions</u>	$\langle \rangle \rangle$
25	of SIF retrieved by IAPCAS/SIF from TanSat and OCO-2 shows the same spatial pattern for all seasons with gridded SIF	
26	difference less than 0.3 W m <sup>-2</sup> µm <sup>-1</sup> sr <sup>-1</sup> , The global distributions also agree, well with the official OCO-2 SIF product with	M
27	difference less than 0.2 W m <sup>-2</sup> $\mu$ m <sup>-1</sup> sr <sup>-1</sup> . The retrieval uncertainty of seasonally gridded TanSat <u>IAPCAS/SIF</u> is less than 0.03	///
28	$W\ m^{-2}\ \mu m^{-1}\ sr^{-1}\ whereas\ the\ uncertainty\ of\ each\ sounding\ ranges\ from\ 0.1\ to\ 0.6\ W\ m^{-2}\ \mu m^{-1}\ sr^{-1}.$ The relationship between	$\langle \rangle$
29	annually-averaged SIF products and FLUXCOM gross primary productivity (GPP) was also estimated for six vegetation types	
30	in a $1^{\circ} \times 1^{\circ}$ grid over the globe, indicating that the SIF data from the two satellites have the same potential in quantitatively	
31	characterizing ecosystem productivity. The spatiotemporal consistency between TanSat and OCO-2 and their comparable data	
32	quality enable joint usage of the two mission products, Data supplemented by TanSat observations are expected to contribute	
33	to the development of global SIF maps with more spatiotemporal detail, which will advance global research on vegetation	$\overline{\ }$
34	photosynthesis.	

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	<b>删除的内容:</b> thatith high signal-to-noise ratio and spectral resolution. The Chinese global carbon dioxide monitoring satellite (TanSat), as its mission,acquires measurements of greenhouse gas column densitiesgreenhouse gas column density The advanced technical characteristics of the hyper-spectrumrating spectrometer (ACGS) onboard TanSat enable SIF retrievals from spacebservations in the O <sub>2</sub> -A band. In this study, oneear of SIF data <b>for each sounding</b>			
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#### 108 1 Introduction

109	Terrestrial vegetation ecosystems play a large role in the global carbon cycle through the processes of photosynthesis and	
110	respiration, Incoming radiation is absorbed, reflected, and/or transmitted by plant leaves. A portion of the absorbed radiation	
111	is used by the chlorophyll in plant leaves for carbon fixation, while the rest is either dissipated as heat or re-emitted as solar-	
112	induced chlorophyll fluorescence (SIF) at longer wavelengths (Frankenberg et al., 2011a, 2014). In contrast to the traditional	
113	remotely sensed vegetation indices obtained from some studies (Frankenberg et al., 2011b; Guanter et al., 2014; Li et al., 2018;	
114	Sun et al., 2017a; Yang et al., 2015; Zhang et al., 2014), SIF offers the potential to measure photosynthetic activity and gross	
115	primary production (GPP), due to the strong correlation between these measures (Frankenberg et al., 2011b; Guanter et al.,	
116	2012, 2014). The fluorescence emission adds a low-intensity radiance <u>of</u> less than 10 W m <sup>-2</sup> $\mu$ m <sup>-1</sup> sr <sup>-1</sup> and fills in the solar	
117	absorption features of the reflected spectrum (Frankenberg et al., 2011a). The filling-in effect of the solar lines (Fraunhofer	
118	lines) is the basic principle applied to measure SIF from space using the capabilities of hyperspectral observation (Frankenberg	
119	et al., 2011b; Guanter et al., 2012).	
120	The first attempt of observing SIF from space was performed using images acquired by the Medium Resolution Imaging	
121	Spectrometer (MERIS) onboard the ENVIronmental SATellite (ENVISAT) (Guanter et al., 2007). This led to a new idea for	
122	conducting SIF studies on a global scale. The first global SIF map was retrieved from high-resolution spectra of the	
123	Greenhouse-gases Observing SATellite (GOSAT) (Joiner et al., 2011; Frankenberg et al., 2011b). After that, SIF retrievals	
124	were implemented for a variety of satellite measurements, such as those from the Global Ozone Monitoring Experiment-2	
125	(GOME-2) instruments onboard meteorological operational satellites, SCIAMACHY onboard ENVISAT, and Orbiting	
126	Carbon Observatory-2 (OCO-2) (Joiner et al., 2016; Köhler et al., 2015). The TROPOspheric Monitoring Instrument	
127	(TROPOMI) onboard Sentinel 5 Precursor (S-5P) provides more efficient SIF observations in terms of global coverage and	
128	new opportunities for exploring the application potential of SIF data in the terrestrial biosphere as well as in climate research	
129	(Doughty et al., 2019; Köhler et al., 2018b). Furthermore, an upcoming European Space Agency mission called FLuorescence	
130	EXplorer (FLEX), the first satellite dedicated to SIF observation, will launch in the middle of 2024 (Drusch et al., 2017). Many	
131	studies on SIF applications have been initiated with the accumulation of SIF products in recent years. The responses of satellite-	
132	measured SIF to environmental conditions have been applied to drought dynamics monitoring and regional vegetation water	
133	stress estimation (Lee et al., 2013; Sun et al., 2015; Yoshida et al., 2015). As a proxy of photosynthesis, SIF acts as a powerful	
134	constraint parameter in estimating carbon exchange in an ecosystem between the atmosphere, ocean, and soil; as such, the	
135	analysis of the relationship between SIF and GPP has become an important research topic (Li et al., 2018; Köhler et al., 2018a;	
136	Sun et al., 2017a; Zhang et al., 2018). The strong linear relationship between them paves the way for improving terrestrial	
137	ecosystem model simulations of GPP, along with consequent improvement of global carbon flux estimation (MacBean et al.,	
138	2018; Yin et al., 2020). GPP estimations based on satellite-measured SIF have proven to be an effective method validated by	
139	in-situ flux observations (Joiner et al., 2018; Qiu et al., 2020). However, uncertainty in the factors that determine the	
140	relationship between SIF and GPP still exists and is a key limitation in the application of SIF to flux estimation. Based on	

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154 multi-satellite SIF products, eddy covariance flux tower observations, and ecological models, the relationship between SIF and

155 GPP under different environmental conditions has been discussed in a number of studies to analyze the dominant factors for

156 the growing status of different biomes, such as temperature, soil moisture, and vegetation types (Chen et al., 2020; Doughty et

157 al., 2019; Li et al., 2020; Qiu et al., 2020; Yin et al., 2020).

158 The Chinese global carbon dioxide monitoring satellite (TanSat) was launched in December 2016. Aiming at acquiring CO<sub>2</sub> 159 concentrations similar to OCO-2, TanSat flies in a sun-synchronous orbit at approximately 700 km height with a 16-day repeat cycle and an equator crossing time of ~1:30 p.m. local time (Cai et al., 2014; Liu et al., 2018; Yang et al., 2018). Onboard 160 161 TanSat, the hyperspectral Atmospheric Carbon-dioxide Grating Spectrometer (ACGS) is designed to separately record solar backscatter spectra in three channels centered at 0.76 µm (O<sub>2</sub>-A band), 1.61 µm (weak CO<sub>2</sub> absorption band), and 2.06 µm 162 163 (strong CO2 absorption band). Many Optimal Estimation Method (OEM) full physics retrieval algorithms have been developed 164 and applied for the total column-averaged dry air CO2 mole fraction (XCO<sub>2</sub>) retrievals (Bösch et al., 2006; O'Dell et al., 2012; 165 Reuter et al., 2010; Yang et al., 2015b; Yoshida et al., 2011, 2013). The Institute of Atmospheric Physics Carbon Dioxide 166 Retrieval Algorithm for Satellite Remote Sensing (IAPCAS) algorithm has been applied for TanSat XCO2 retrievals (Yang et 167 al., 2018; Yang et al., 2021) and was also previously tested on spectra from the GOSAT and OCO-2 missions (Yang et al., 168 2015b). However, the fluorescence feature causes substantial biases when retrieving surface pressure and scattering parameters 169 from the O<sub>2</sub>-A band, and the associated errors propagate into the XCO<sub>2</sub> retrievals. In previous XCO<sub>2</sub> retrievals, the surface 170 emissions were well modeled as a continuum offset of the O2-A band to reduce errors (Frankenberg et al., 2011a, 2012; Joiner 171 et al., 2012). For TanSat, its high spectral resolution of ~0.044 nm and a signal-to-noise ratio of ~360 in the O<sub>2</sub>-A band makes 172 it possible to obtain SIF, with a spatial resolution of  $2 \text{ km} \times 2 \text{ km}$  in nadir mode (Liu et al., 2018). 173 Various approaches have been used to infer SIF from satellite measurements (Frankenberg et al., 2011b, 2014a, 2014b; Guanter et al., 2007, 2012, 2015; Joiner et al., 2011, 2013, 2016; Köhler et al., 2015, 2018b). The SIF signal induces a filling-in effect 174

175 of solar lines, which can be used for SIF retrieval, as the fractional depth of solar Fraunhofer lines does not change during 176 radiation transmission in the atmosphere. To be able to measure the filling-in features from SIF, high-resolution spectra are 177 required to describe subtle changes in the spectral absorption lines. Given highly resolved spectral features, a method was 178 developed based on solar line fitting and the Beer-Lambertian law. This method is robust and accurate when the spectrum is 179 out of the influence of telluric absorptions, even in the presence of aerosols (Frankenberg et al., 2011a; Joiner et al., 2011); in 180 the current study, this method was applied to develop the IAPCAS/SIF algorithm. Another SIF retrieval method is the data-181 driven algorithm based on the singular value decomposition (SVD) technique (Joiner et al., 2011; Guanter et al., 2012), which has been broadly applied to GOSAT, OCO-2, TanSat and TROPOMI (Joiner et al., 2011; Guanter et al., 2012, 2015; 182 183 Frankenberg et al., 2014a; Du et al., 2018; Köhler et al., 2018b). In the data-driven method, the spectrum is represented as a linear combination of the SIF signal and several singular vectors that are trained from non-fluorescent scenes by SVD; thus, 184 the SIF signal can be obtained with linear least-squares fitting (Du et al., 2018; Guanter et al., 2012). The first TanSat SIF 185 map was obtained by the SVD method (Du et al., 2018). In a previous study, a new TanSat SIF product retrieved by 186 IAPCAS/SIF algorithm was introduced and the two kinds of TanSat SIF products by IAPCAS/SIF and the SVD methods were 187

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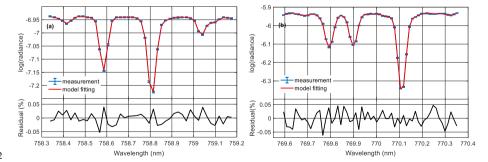
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- 206 compared (Yao et al., 2021). The preliminary comparison between the two TanSat SIF products showed that the two SIF
- 207 products share a similar global pattern and signal magnitude for all seasons while different biases still exist in four seasons
- 208 (Yao et al., 2021). The different biases in the four seasons may be caused by the different training samples of the SVD method,
- 209 which indicates that the training samples have a significant impact on the retrieval results. In order to obtain stable SIF data
- 210 products from TanSat and other subsequent satellite missions, it is particularly important to establish a stable and high-
- 211 precision SIF inversion algorithm. To further validate the IAPCAS/SIF algorithm and to test the potential for synergistic,
- 212 multi-satellite SIF analysis, in this study, we detail the IAPCAS/SIF algorithm for TanSat and we compare the SIF products
- 213 from TanSat and OCO-2 for a range of spatiotemporal scales.

# 214 2 Data and retrieval algorithm

#### 215 2.1 Retrieval Principle and Method

- 216 We used TanSat version 2 Level 1B (L1B) nadir-mode earth observation data in the retrieval process. The measurements
- $217 \quad \text{covered the period from March 2017 to February 2018. Polarized radiance in the O_2-A band with a spectral resolution of 0.044$
- 218 nm was provided in the L1B data, and two micro-windows near 757 nm (758.3-759.2 nm) and 771 nm (769.6-770.3 nm) were
- 219 chosen to retrieve top-of-atmosphere (TOA) SIF while avoiding the contamination from strong lines of atmospheric gas
- 220 absorption. The retrieval was independent for each micro-window as shown in Figure 1. To avoid duplication of information,
- 221 we use the SIF product at 757 nm as the example in the analysis.



# 222

Figure 1: The fitted spectra and residuals for the (a) 757 nm and (b) 771 nm micro-windows of TanSat measurement. The error bar of the measured spectra depicts the estimated precision of each TanSat sounding.

- 225
- 226 Filling-in on solar lines by chlorophyll fluorescence in the O2-A band can be detected in the hyperspectral measurements from
- 227 TanSat. This effect on spectral radiance is different from the impact of atmospheric and surface processes, e.g., scattering and
- 228 absorption. For example, scattering by aerosols and clouds does not change the relative depth of clear solar lines, unlike the

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237	SIF emission signal.	We applied the differential	optical absorption s	pectroscopy (DOAS)	) technique to IAPCAS/SIF algorith	m

- 238 for TanSat measurement (Frankenberg, 2014b; Sun et al., 2018).
- 239 The TOA spectral radiance  $(L_{TOA}^{\lambda})$  at wavelength  $\lambda$  can be represented as follows:

240 
$$L_{TOA}^{\lambda} = I_{t}^{\lambda} \cdot \mu_{0} \cdot (\rho_{0}^{\lambda} + \frac{\rho_{s}^{\lambda} \cdot T_{t}^{\lambda} \cdot T_{t}^{\lambda}}{\pi}) + F_{TOA}^{\lambda}$$

(1)

(2)

(3)

241 where  $I_t^{\lambda}$  is the incident solar irradiance at the TOA,  $\mu_0$  is the cosine of the solar zenith angle (SZA),  $\rho_0^{\lambda}$  is atmospheric path

242 reflectance,  $\rho_s^{\lambda}$  is surface reflectance, and  $T_1^{\lambda}$  and  $T_1^{\lambda}$  are the total atmospheric transmittances along the light-path in the

243 downstream and upstream directions, respectively.  $F_{TOA}^{\lambda}$  is the SIF radiance at TOA.

244 The first term on the right of Eq. (1) represents the transmission process of solar radiance. In the micro-windows used in SIF

retrieval, gas absorption is very weak and smooth, and hence, the atmosphere term  $\mu_0 \cdot (\rho_0^{\lambda} + \frac{\rho_s^{\lambda} \cdot T_i^{\lambda} \cdot T_i^{\lambda}}{\pi})$  can be simplified to a

246 low-order polynomial  $\sum_{i=0}^{n} a_i \cdot \lambda^i$  that varies with  $\lambda$  (Joiner et al., 2013; Sun et al., 2018); this is always valid as long as the

247 spectrum fitting range is out of sharp atmospheric absorptions. Then Eq. (1) could be represented as:

248  $L^{\lambda}_{TOA}(F^{\lambda}_{TOA}, \boldsymbol{a}) = < I^{\lambda}_{t} > \sum_{i=0}^{n} a_{i} \cdot \lambda^{i} + F^{\lambda}_{TOA}$ 

249	where $<>$ denote the convolution with the ISRF from line-by-line spectra, and the coefficient vector $a$ determines the
250	wavelength dependence polynomial for the atmosphere term.

251 To facilitate the extraction of SIF signals, the radiance is normalized to the continuum level radiance and the relative

252 contribution of SIF to the continuum level radiance  $F_s^{rel}$  is defined. In the micro-window, SIF was regarded as a constant signal

253 due to its small changes. When the spectral radiance measurement was converted to logarithmic space, the forward model was

254 expressed as:

255  $f(F_s^{rel}, \boldsymbol{b}) = log(\langle I_t + F_s^{rel} \rangle) + \sum_{i=0}^n b_i \cdot \lambda^i$ 

256 Where  $I_{t}$  is a normalized disk-integrated solar transmission model. The vector p consists of the polynomial coefficients p

and we used a second-order polynomial (i = 0, 1, 2) in the retrieval,

258 Although the atmospheric gas absorption was very weak in the micro-window, the weak absorption and the far-wing effects

259 (O<sub>2</sub> lines) can still change spectral features, which induces errors in spectrum fitting. In other <u>physics</u>-based retrievals, the

surface pressure data of the European Centre for Medium-Range Weather Forecasts (ECMWF) together with topographic data

- 261 are usually used as the true surface pressure to simulate the atmospheric transmission in the range of the O2-A band. However,
- there is still a difference between the true surface pressure and the model surface pressure, so we introduced a factor here to
- 263 reduce the influence, of the inaccurate surface pressure. In the IAPCAS/SIF algorithm, we use, the ECMWF interim surface

264 pressure  $(0.75^{\circ} \times 0.75^{\circ})$  to estimate O<sub>2</sub> absorption first and then <u>modify</u> the absorption feature by a scale factor. The scale

265 factor is obtained simultaneously in SIF retrieval to reduce the error induced by the uncertainty in surface pressure. As

described by Yang (2020), there is also a continuum feature in TanSat L1B data that needs to be considered for the high-quality

267 fitting of the O<sub>2</sub>-A band. However, in this study, this continuum feature was not corrected, as the impact of such a smooth

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296 continuum variation in the micro-window is weak and the polynomial continuum model is capable of compensating for most 297 of this effect.

298 The state vector includes the relative SIF signal  $F_s^{rel}$ , a wavenumber shift, the scale factor for the O<sub>2</sub> column absorption, and

299 coefficients of the polynomial. The continuum level radiance I<sub>cont</sub> within the fitting window is calculated using the radiance

300 outside the absorption features in the micro-window and is then used for the actual SIF signal calculation thus:  $F = F_{c}^{rel} \cdot I_{cnnt}$ .

301 In the IAPCAS/SIF algorithm, we used an OEM for state vector optimization in the retrieval process. <u>Compared to the IAPCAS</u>

302 XCO<sub>2</sub> retrieval, the IAPCAS/SIF retrieval employs a state vector with fewer elements and a much simpler forward model, so

303 there is no need to perform complex radiative transfer calculations. Considering the low complexity of SIF retrieval, the Gauss-

304 Newton method was applied iteratively to find the optimal solution.

# 305 2.2 Bias Corrections

306 A systematic error remains in the raw SIF retrieval output if no bias correction is performed; similar results have been reported 307 in GOSAT and OCO-2 SIF retrieval studies (Frankenberg et al., 2011a, 2011b; Sun et al., 2018). This is because the SIF signal 308 is weak (e.g., typically ~1-2% of the continuum level radiance), which means that even a small issue in the measurement, such as a zero-offset caused by radiometric calibration error, could induce significant bias. Unfortunately, the lack of knowledge on 309 310 in-flight instrument performance makes it difficult to perform a direct systematic bias correction in the measured spectrum. 311 The bias was considered to be related to the continuum level radiance in the previous works. To get the relationship between 312 the continuum level radiance and the bias, we calculated the mean bias for continuum level radiance at the interval of 5 W m<sup>-2</sup> 313 µm<sup>-1</sup> sr<sup>-1</sup> from all non-fluorescence measurements, and then a piecewise linear function fit was applied to describe the 314 relationship between the continuum level radiance and the biases 315 The non-fluorescence soundings that were used in the bias estimation were based on the dataset "sounding landCover" in 316 TanSat L1B data. This dataset depends on the MODIS land cover product and provides a scheme consisting of 17 land cover 317 classifications defined by the International Geosphere-Biosphere Programme. The measurements marked as "snow and ice," 318 "barren," and "sparsely vegetated" were chosen to estimate the bias. Calibrations compensated for most of the instrument 319 degradations, but this alone was not perfect. To reduce the impact from the remaining minor discrepancies, we built the bias 320 correction function daily to obtain bias for each sounding via interpolation of the continuum level radiance (Sun et al., 2017b,

321 2018).

322 The bias curves shown in Figure 2 differ significantly between TanSat and OCO-2. This is mostly due to the differences in

323 instrument performance and radiometric calibration. In general, the TanSat bias curves exhibited two peaks at radiance levels

324 of approximately 40 and 125 W m<sup>-2</sup>  $\mu$ m<sup>-1</sup> sr<sup>-1</sup>, separately, and most biases were larger than 0.015. For OCO-2, the curves

325 dropped sharply at low radiance levels, reaching the valley at a radiance level of approximately 40 W m<sup>-2</sup>  $\mu$ m<sup>-1</sup> sr<sup>-1</sup>, and then

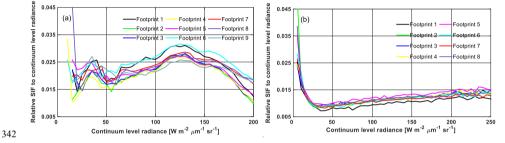
326 increased slowly with the radiance level.

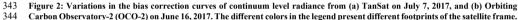
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	used to estimate the bias. The bins have a continuum level radiance					
	interval of 5 W m <sup>-2</sup> µm <sup>-1</sup> sr <sup>-1</sup> . In each bin, the mean bias was					
	estimated using all non-fluorescence measurements, and a piecewise					
	linear function was built from the mean bias of each continuum level					
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345 2.3 Data Quality Controls

Only data that passed quality control were used in further applications. There were two data quality control processes for the SIF products: pre-screening and post-screening. Pre-screening focused mainly on cloud screening; only cloud-free measurements were used in SIF retrieval. A surface pressure difference (SPD), defined as:

$$349 \quad \Delta P_0 = |P_{retrieval} - P_{ECMWF}| \tag{3}$$

350 was used to evaluate cloud contamination along with a chi-square test

$$351 \quad \chi^2 = \sum \frac{(y_{sim} - y_{obs})^2}{y_{noise}^2}$$

352 where ysim, yobs, and ynoise represent the model fitting spectrum, observation spectrum, and spectrum noise, respectively. Pretrieval is the apparent surface pressure obtained from O2-A band surface pressure retrieval, assuming a Rayleigh-scattering 353 354 atmosphere. PECMWF is the surface pressure data from the ECMWF interim (0.75° × 0.75°) reanalysis data product (Dee et al., 355 2011) which is interpolated to the sounding location and corrected for elevation differences with the Shuttle Radar Topography 356 Mission Global 30 Arc-Second Elevation digital elevation model (DOI: 10.5067/MEaSUREs/SRTM/SRTMGL30.002). A 357 "cloud-free" measurement was required to simultaneously satisfy an SPD of less than 20 hPa and a  $\chi^2$  value of less than 80. Here, post-screening was applied to filter out "bad" retrievals; this screening process involved the following steps: (1) SIF 358 359 retrievals with reduced  $\chi^2$  ( $\chi^2_{red}$ ) values ranging from 0.7 to 1.3 were considered "good" fitting, (2) continuum level radiance outside the range of  $15 \sim 200 \text{ W m}^{-2} \mu \text{m}^{-1} \text{ sr}^{-1}$  was screened out to avoid scenes too bright or too dark, and (3) soundings with 360 361 the SZA higher than 60° were also filtered out.

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# 363 2.4 IAPCAS versus IMAP-DOAS OCO-2 SIF Retrieval

364 Before applied to TanSat retrievals, we tested the IAPCAS/SIF algorithm on the OCO-2 L1B data first 365 (OCO2\_L1B\_Science.8r) and then compared the retrieval results with the OCO-2 L2 Lite SIF product (OCO2 Level

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369 2\_Lite\_SIF.8r) retrieved by the Iterative Maximum A Posteriori-Differential Optical Absorption Spectroscopy (IMAP-DOAS)

algorithm (Frankenberg, 2014b). The Lite product provides the SIF value for each sounding and hence the SIF comparison

371 could be performed on the sounding scale for each month.

372 Table 1 displays the relationship of OCO-2 SIF values between the IAPCAS/SIF and IMAP-DOAS at 757 nm micro-window

373 for each month. Overall, the two SIF products were in good agreement. The linear fitting of the two SIF products suggests that

374 they are highly correlated, as indicated by the strong linear relationship with  $R^2$  mostly larger than 0.85 and the root mean

square error (RMSE) of about 0.2 W m<sup>-2</sup> µm<sup>-1</sup> sr<sup>-1</sup>. Good consistency between the two SIF products implies the reliability of

376 the IAPCAS/SIF algorithm; thus, it was further applied to TanSat SIF retrieval. However, there was still a small bias in the

377 comparisons, which was due, most likely, to the impact of differences in the bias correction method, retrieval algorithm, and

378 fitting window.

Table 1: Summary of the relationship between the JAPCAS OCO-2 and JMAP-DOAS OCO-2 solar-induced chlorophyll fluorescence
 (SIF) products at 757nm micro-window.

month	Number of soundings	Slope	Intercept	$\mathbb{R}^2$	RMSE/ W m <sup>-2</sup> µm <sup>-1</sup> sr <sup>-1</sup>
2017/03	1097277	0.85	0.034	0.86	0.18
2017/04	1119464	0.86	0.045	0.87	0.19
2017/05	1054235	0.88	0.041	0.88	0.19
2017/06	1014848	0.91	0.032	0.90	0.19
2017/07	965309	0.92	0.011	0.91	0.19
2017/09	211219	0.88	0.005	0.81	0.23
2017/10	473359	0.88	0.031	0.88	0.17
2017/11	579009	0.87	0.022	0.85	0.19
2017/12	645134	0.87	0.020	0.88	0.16
2018/01	788655	0.87	0.019	0.88	0.17
2018/02*	629995	0.86	0.024	0.87	0.18

381 \* Due to the lack of OCO-2 measurements in August 2017, the comparison is only performed for 11 months.

### 382 3 Results and Discussion

#### 383 3.1 Comparison between TanSat and OCO-2 SIF Measurements

384 The comparison between TanSat and OCO-2 SIF measurements is a useful and powerful method for further verification of the

385 IAPCAS/SIF algorithm. The reason for adopting OCO-2 data is that OCO-2 and TanSat have similar observation modes,

386 including scanning method, transit time, spatial resolution, spectral resolution, and spectral range. The similarities mean that

387 the SIF product from the two satellite missions can be directly compared. Directly comparing OCO-2 and TanSat SIF

measurements could provide information on joint data application at the sounding scale for further studies. However, an

389 identical sounding overlap barely exists because the two satellites often have different nadir tracks on the ground, which is

induced by the different temporal and spatial intervals of the two satellite missions. Fortunately, the ground tracks of the two

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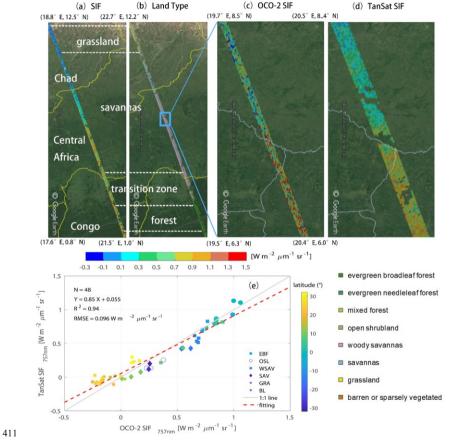
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399 satellites were relatively close from April 17 to April 23, 2017. A couple of overlapping orbits were found in the measurements 400 obtained from Africa with the orbit number of 1733 from TanSat and 14890a from OCO-2 (Figure 3). In the comparison, the 401 OCO2 Level 2 Lite SIF.8r product was used to present the SIF emission over the study area. These overlapping 402 measurements encompassed multiple land cover types, in which the SIF varied within an acceptable time difference (<5 min). 403 Overall, measurements from the two satellites indicated SIF variation with land cover type. The SIF emission over evergreen 404 broadleaf forests was larger than that over savannas, and grasslands exhibited the lowest SIF emission in April (Figure 3a,b). The mean SIF emission over evergreen broadleaf forests was approximately 0.9-1.1 W m<sup>-2</sup> µm<sup>-1</sup> sr<sup>-1</sup>, whereas those over 405 savannas and grasslands were 0.5-0.7 W m<sup>-2</sup>  $\mu$ m<sup>-1</sup> sr<sup>-1</sup> and less than 0.1 W m<sup>-2</sup>  $\mu$ m<sup>-1</sup> sr<sup>-1</sup>, respectively (Figure 3c.d). 406 Furthermore, we also found a significant difference in the SIF emission intensity over tropical savannas, which was observed 407 by both satellites (Figure 3c,d). 408

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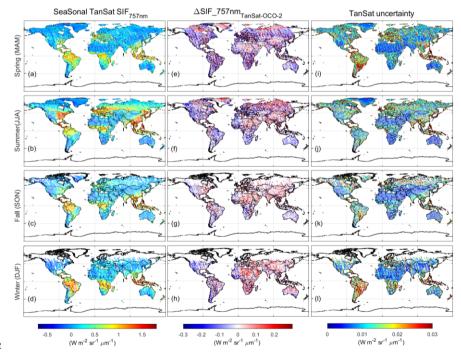
412 Figure 3: Overlapping orbits of TanSat and OCO-2 on April 19, 2017 over Africa displayed in Google Earth, (a) the SIF 413 measurements from both satellites and (b) the footprint land cover type were compared. Compared to OCO-2, TanSat has a wider 414 swath width. A zoom-in view over savannas shows variations in the SIF signal measured by (c) OCO-2 and (d) TanSat. The land 415 surface image shown in Google earth is provided by Landsat/Copernicus team. Following the International Geosphere-Biosphere 416 Programme classification scheme, the vertical legend on the bottom right corner depicts the land cover type that occurs in the study 417 area. The middle horizontal color bar represents the intensity of the SIF radiance. (e) Small-area SIF comparison between OCO-2 418 and TanSat; each data point represents the mean SIF of a degree in latitude (colors) along the track. The marker legend that is 419 shown on the bottom right of the plot indicates the dominant land cover (defined as the majority land cover type of each sounding) 420 in each small area. There are six land cover types including evergreen broadleaf forest (EBF), open shrubland (OSL), woody savanna 421 (WSAV), savanna (SAV), grassland (GRA), and barren land (BL). The red dashed line represents the linear fit between the two SIF 422 products with statistics shown in the upper left of the plot. The gray line indicates a 1:1 relationship for reference.

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425 Because the footprint sizes of the two satellites are different, it is difficult to make a direct footprint-to-footprint comparison. 426 Therefore, we made the comparison between the two satellite measurements based on a small area average. Each small area spans a degree in latitude and continues along the track. The small area-averaged SIF comparison is shown in Figure 3e. The 427 results indicate good agreement, with an R<sup>2</sup> of 0.94 and an RMSE of 0.096 W m<sup>-2</sup> µm<sup>-1</sup> sr<sup>-1</sup>. Additional ground-based SIF 428 429 measurement setups (Guanter et al., 2007; Liu et al., 2019; van der Tol et al., 2016; Yang et al., 2015a; Yu et al., 2019) should 430 allow for direct evaluation of satellite retrieval accuracy in the future.

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432

433 Figure 4: Global TanSat SIF (left, a-d), differences between TanSat and IAPCAS OCO-2 SIF values (middle, e-h), and the grid-cell retrieval uncertainty estimated from TanSat (right, i-l) at 1° × 1° spatial resolution. The maps in each row represent a Northern

434 435 Hemisphere season, i.e., spring (MAM), summer (JJA), fall (SON), and winter (DJF).

437 Figure 4 shows the global SIF comparison between IAPCAS/SIF retrieved from OCO-2 and TanSat; this comparison is only performed at  $1^{\circ} \times 1^{\circ}$  spatial resolution. In general, the difference in SIF globally is mostly less than 0.3 W m<sup>-2</sup>  $\mu$ m<sup>-1</sup> sr<sup>-1</sup> for 438 439 all seasons, and on average, the smallest difference appears in fall. There are regional biases observed in North Africa, South 440 Africa, South America, and Europe in all seasons except fall. This is mainly caused by the differences in instrument 441 performance between TanSat and OCO-2, such as the Instrument Spectral Respond and the Signal-to-Noise. The instrument 442 performance difference is represented by the different structural characteristics of the bias curves. The bias correction 443 compensates for most of the bias caused by instrument performance; however, small biases could remain. Furthermore, the 444 hundreds of kilometers of distance between the OCO-2 and TanSat footprints, for example, over different vegetation regions, 445 will also cause some measurement discrepancies. The global distribution of the two satellites was also compared with the 446 official OCO-2 SIF data on the global scale, the results show that the difference between the retrieved SIF maps and the official map is less than 0.2 W m<sup>-2</sup> µm<sup>-1</sup> sr<sup>-1</sup>, indicating that the retrieved SIF data from OCO-2 and TanSat both have good SIF 447 448 characterization capabilities on a global scale. The uncertainty  $\sigma$  of each sounding was estimated to validate SIF reliability and is provided in the product.  $\sigma$  is derived from the retrieval error covariance matrix,  $S_e = (K^T S_0^{-1} K)^{-1}$ , where K is the Jacobian 449 450 matrix from the forward model fitting and  $S_0$  is the measurement error covariance matrix that is calculated from the instrument spectrum noise. In general,  $\sigma$  ranges from 0.1 to 0.6 W m<sup>-2</sup>  $\mu$ m<sup>-1</sup> sr<sup>-1</sup> for both TanSat and OCO-2 measurements in the 757 451 452 nm fitting window, which is of a similar magnitude and data range as those of previous studies (Du et al., 2018; Frankenberg 453 et al., 2014a). Meanwhile, the standard error of the mean SIF in each grid  $\sigma_{meas}$  was estimated to represent the gridded retrieval error and natural variability, which is calculated from TanSat SIF values with  $\sigma_{meas} = \frac{\sigma_{std}}{\sqrt{n}}$  and  $\sigma_{std} = \sqrt{\frac{\sum_{i=1}^{n} (SIF_i - \overline{SIF})^2}{n}}$ , where 454  $\sigma_{std}$  represents the standard deviation of the grid cell with n soundings, SIF<sub>i</sub> is the retrieved SIF values of each sounding, 455 456 and  $\overline{SIF}$  is the mean SIF value for all measurements in the grid. As depicted in the right column of Figure 4, the  $\sigma_{meas}$  of each 457 grid cell is much lower than the precision of a single sounding. The  $\sigma_{meas}$  for South America is larger than that for any other region on the globe (Figure 4i-l). This is similar to that of OCO-2 SIF retrieval and caused by fewer effective measurements 458 459 due to the South Atlantic Anomaly (Sun et al., 2018). The difference in SIF emission values between the two satellites indicates 460 that the synergistic use of two satellite SIF products still requires analysis of the impact of instrument differences, although 461 the two satellite SIF products share the same spatiotemporal pattern on a global scale.

# 462 3.2 SIF Global Distribution and Temporal Variation

463 The SIF emission intensity reflects the growth status of vegetation, and hence, the overall global vegetation status can be

- represented by global SIF maps for each season. TanSat SIF over a whole year's cycle, from March 2017 to February 2018, is represented seasonally as a  $1^{\circ} \times 1^{\circ}$  grid spatially. The seasonal variation in SIF emission is clear in the Northern Hemisphere,
- 466 i.e., it is enhanced from spring to summer and then decreases (Sun et al., 2018).
- 467 In general, the SIF emission varied with latitude and the vegetation-covered areas near the equator maintained a continuous
- 468 SIF emission throughout the year. Large SIF emissions in the Northern Hemisphere, above 1.5 W m<sup>-2</sup>  $\mu$ m<sup>-1</sup> sr<sup>-1</sup>, mostly from

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obvious SIF emission of 1-1.2 W m<sup>-2</sup> µm<sup>-1</sup> sr<sup>-1</sup> observed over Central Europe and northeastern China during the summer. In 475 476 these regions, croplands and deciduous forests contribute to SIF emissions. In the Southern Hemisphere, the strongest SIF emission occurred in the Amazon, with a level of approximately 1-2 W m<sup>-2</sup> µm<sup>-1</sup> sr<sup>-1</sup> in DJF (Northern Hemisphere winter), 477 where there is an evergreen broadleaf rainforest. Africa, which is covered by evergreen broadleaf rainforests and woody 478 savannas, had an average SIF value of 0.7-1.5 W m<sup>-2</sup> µm<sup>-1</sup> sr<sup>-1</sup> during the year. 479 480 The SIF-GPP relationship over different vegetation types was also investigated by comparing the annual mean satellite SIF 481 measurements with the FLUXCOM GPP (Jung et al., 2020; Tramontana et al., 2016) dataset in a  $1^{\circ} \times 1^{\circ}$  grid over the globe. 482 The FLUXCOM GPP dataset used in the study comprises monthly global gridded flux products with remote sensing and 483 meteorological/climate forcing (RS+METEO) setups, which are derived from mean seasonal cycles according to MODIS data and daily meteorological information (Jung et al., 2020; Tramontana et al., 2016). In the correlation analysis, the high spatial 484 485 resolution  $(0.5^{\circ} \times 0.5^{\circ})$  of the FLUXCOM GPP was first resampled to  $1^{\circ} \times 1^{\circ}$  to keep the same temporal-spatial scale of SIF and GPP data. The satellite-measured SIF is an instantaneous emission signal that varies with incident solar radiance within 486 the day. To reduce the differences caused by the observation time and SZA at different latitudes, we applied a daily adjustment 487 488 factor to convert the instantaneous SIF emission into a daily mean SIF (Du et al., 2018; Frankenberg et al., 2011b; Sun et al., 2018). The daily adjustment factor d is calculated as follows: 489

the eastern U.S., southeast of China, and southern Asia in summer, were due to the large areas of cropland. There was also an

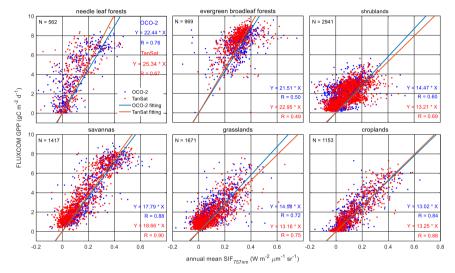
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$$d = \frac{\int_{t=t_0-12h}^{t=t_0+12h} \cos(SZA(t)) \cdot dt}{\cos(SZA(t_0))}$$

491 where  $t_0$  is the observation time in fractional days and SZA(t) is a function of latitude, longitude, and time for calculating the 492 SZA of the measurements. The annual averaged SIF is calculated from the daily mean SIF. To evaluate the relationship

(5)

493 between SIF and GPP on the periodic scale of vegetation growth status, annually-averaged data were used in the regression 494 fitting analysis.



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Figure 5: Relationship between annual mean SIF and FLUXCOM gross primary production (GPP) from March 2017 to February
 2018. Blue and red dots represent OCO-2 and TanSat SIF grids, respectively. Fitted lines and statistics for OCO-2 and TanSat are
 shown in each plot.

499 Figure 5 shows the linear fits for six vegetation types, including needle leaf forest, evergreen broadleaf forest, shrubland, savanna, grassland, and cropland. Recent studies have shown a strong linear correlation between SIF and GPP. The TanSat 500 501 SIF and the OCO-2 official SIF data were used to estimate the SIF-GPP correlation. To make a direct comparison of the 502 relationship between SIF and GPP among various vegetation types, we used non-offset linear fitting to indicate the correlation 503 between satellite SIF and FLUXCOM GPP. For savanna and cropland, there were strong relationships between the mean SIF 504 and GPP with an R-value above 0.84. The fitting results show that the SIF products of the two satellites have similar capabilities in characterizing GPP, especially for the evergreen broadleaf forest, savanna, and cropland, with slopes of approximately 21, 505 18, and 13, respectively. For shrubland and grassland, the slope of OCO-2 SIF with GPP is higher than that of TanSat and has 506 a worse correlation. For forests, OCO-2 SIF presents a better correlation with GPP, especially in the needle leaf forest. As a 507 508 whole, for the same vegetation type, the SIF-GPP correlations for the two satellites are rather similar, indicating that the two 509 satellite SIF products have similar capabilities in characterizing GPP. It shows the strong feasibility of the comprehensive application of different satellite SIF products. For different vegetation types, the SIF-GPP correlations were significantly 510 511 different, indicating the different ability of SIF to characterize GPP of different vegetation. It represents that vegetation type 512 is a key factor in determining the SIF-GPP relationship. The markedly different fitting slopes across various biomes suggest 513 that the application of SIF in GPP estimation needs more detailed analysis although the evidence of the strong linear 514 relationship between them.

#### 515 4 Conclusions

516 In this paper, we introduced the retrieval algorithm IAPCAS/SIF and its application in TanSat and OCO-2 measurements. One 517 year (March 2017-February 2018) of TanSat SIF data was introduced and compared with OCO-2 measurements in this study. 518 The TanSat and OCO-2 SIF products based on the IAPCAS/SIF algorithm are available on the Cooperation on the Analysis 519 of carbon SAtellites data (CASA) website, www.chinageoss.org/tansat. Comparing TanSat and OCO-2 measurements directly, 520 using a case study, and indirectly, with global 1°×1° grid data, showed consistency between the two satellite missions, 521 indicating that the coordinated usage of the two data products is possible in future studies. The correlation analysis between 522 SIF and GPP further verified the feasibility of the synergistic application of SIF products from different satellite missions. 523 Meanwhile, it should be noticed that the difference in the ability of satellite SIF products to characterize different vegetation 524 types in data applications. With more satellites becoming available for SIF observations, space-based SIF observations have 525 recently expanded in range to provide broad spatiotemporal coverage. The next-generation Chinese carbon monitoring satellite 526 (TanSat-2) is now in the preliminary design phase, which is designed to be a constellation of six satellites to measure different 527 kinds of greenhouse gases and trace gases in a more efficient way, including CO2, CH4, CO, NOx, as well as SIF. SIF 528 measurements from TanSat-2 will provide global data products over broader coverage areas with less noise. The improvement 529 in the spatiotemporal resolution of SIF data will benefit GPP predictions based on the numerous studies of the linear 530 relationship between SIF and GPP. In future work, the measurement accuracy should be validated directly using ground-based 531 measurements to ensure data quality.

# 532 Data availability

533 The SIF products of TanSat and OCO-2 by IAPCAS/SIF algorithm are available on the Cooperation on the Analysis of carbon

534 SAtellites data (CASA) website (<u>http://www.chinageoss.cn/tansat/index.html</u>).

#### 535

#### 536 Author contributions

537 L.Y. and D.Y. developed the retrieval algorithm, designed the study, and wrote the paper. Y.L. led the SIF data process and

538 analysis. Y.L., D.Y., Z.C., and J.W. contributed to manuscript organization and revision. C.L. and Y.Z. provided information

539 on the TanSat instrument performance. L.T. provided TanSat in-flight information. M.W. and S.W. provided information on 540 the scientific requirement for data further application. N.L. and D.L. led the TanSat data application. Z.Y. led the TanSat in-

541 flight operation.

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#### 548 Competing interests

549 The authors declare that they have no conflict of interest.

#### 550 Acknowledgments

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