

First Investigation of the Relationship Between Solar-Induced Chlorophyll Fluorescence Observed by TanSat and Gross Primary Productivity

Shanshan Du , Liangyun Liu , Xinjie Liu , and Jidai Chen 

Abstract—Reliable estimation of gross primary production (GPP) of terrestrial ecosystems is crucial in the global carbon cycle and ecosystem functioning studies. Solar-induced chlorophyll fluorescence (SIF) has emerged as an unprecedented proxy for terrestrial GPP estimation. TanSat SIF with a 2-km fine spatial resolution provides an excellent opportunity to investigate the relationships of satellite SIF and eddy covariance (EC) GPP at ecosystem or site scale, while has not been investigated. In this article, we investigated the relationship between TanSat SIF and EC GPP based on flux tower sites encompassing different biomes over the globe. TanSat SIF exhibited strong relationships with EC GPP at Fe and KI bands for instantaneous and daily timescales. The correlations between EC GPP and TanSat SIF ($R^2 = 0.61$) were much better than moderate resolution imaging spectroradiometer (MODIS) bidirectional reflectance distribution function (BRDF)-corrected vegetation indices (VIs) ($R^2 = 0.48$ – 0.58). Further comparisons between SIF and GPP with absorbed photosynthetically active radiation (APAR) and two environmental factors (fTmin and fVPD) showed that SIF responded to APAR and was similarly affected by environmental factors as GPP. GPP derived from SIF ($R^2 = 0.64$) also performed slightly better than enhanced vegetation index and near-infrared reflectance of vegetation and even light use efficiency MODIS GPP algorithm ($R^2 = 0.58$ – 0.60). Therefore, our results demonstrated the feasibility of SIF on estimating GPP at sites or ecosystem levels; in addition, incorporating TanSat SIF with other satellite SIF products will open a new era for carbon cycling and ecosystem functioning studies.

Index Terms—Gross primary productivity, moderate resolution imaging spectroradiometer (MODIS), solar-induced chlorophyll fluorescence (SIF), tanSat.

I. INTRODUCTION

ESTIMATING terrestrial vegetation photosynthesis is significant in understanding the global carbon cycle and monitoring ecosystem productivity [1]–[3]. Reflectance-based vegetation indices (VIs), such as normalized difference vegetation

index (NDVI) and enhanced vegetation index (EVI), are widely used in regional and global vegetation gross primary productivity (GPP) estimation [4]–[6]. However, reflectance-based VIs can only reflect vegetation canopy structure variations; they cannot reveal a photosynthetic capacity, which shows large uncertainties on a small temporal scale and interannual variations [7]. Over the past decade, solar-induced chlorophyll fluorescence (SIF) has been deemed as an alternative proxy for estimating terrestrial GPP due to its close link to photosynthesis [8]–[11]. SIF is essentially an energy flux emitted by plant chlorophyll molecules under natural sunlight, which covers the wavelength range of ~ 650 – 800 nm, with two peaks at ~ 683 and 740 nm. Three different pathways are mainly included when plant chlorophyll molecules absorb light energy: nonphotochemical quenching, photochemistry, and re-emitted as SIF [12], [13]. Consequently, compared with the traditional VIs, SIF shows a close physiological correlation with the photosynthesis status of vegetation [14], [15].

Although numerous studies have demonstrated the significant relationships between SIF and GPP at different spatial and temporal scales using ground-based [8], [16]–[20], airborne-based, and space-borne [9], [11], [21]–[24] remotely sensed SIF observations with gridded GPP or eddy covariance (EC) tower-based GPP measurements, directly employing SIF to estimate global GPP is still challenging. Generally, most ecosystems are homogeneous at the limited spatial scales of hundreds of meters or a few kilometers [25], [26]. The effects of vegetation ecosystem, plant biomes, canopy structure, and even bioclimatic factors on the relationships between SIF and GPP at different temporal and spatial scales require in-depth investigation. To date, numerous atmospheric satellites or sensors have emerged with the potential of global SIF observations from space. Previous studies have successfully obtained global satellite-derived SIF measurements based on the Global Ozone Monitoring Experiment-2 (GOME-2) [27], [28], Scanning Imaging Absorption spectrometer for Atmospheric CHartographY (SCIAMACHY) [29], [30] and Greenhouse Gases Observing Satellite (GOSAT) [31]–[33] observations. However, the coarse spatial resolution of these SIF measurements has hindered GPP evaluation using SIF as there is a spatial mismatch between the observation footprints of a satellite and EC tower. The launch of TROPospheric Monitoring Instrument (TROPOMI) [34]–[36] ($3.5 \text{ km} \times 7 \text{ km}$) and Orbiting Carbon Observatory (OCO-2)

Manuscript received August 11, 2021; revised October 17, 2021 and November 10, 2021; accepted November 12, 2021. Date of publication November 16, 2021; date of current version December 2, 2021. This work was supported in part by the Key Research Program of the Chinese Academy of Sciences under Grant ZDRW-ZS-2019-1, in part by the National Key Research and Development Program of China under Grant 2017YFA0603001 and in part by the National Natural Science Foundation of China under Grant 41871239. (Corresponding author: Liangyun Liu.)

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This article has supplementary downloadable material available at <https://doi.org/10.1109/JSTARS.2021.3128355>, provided by the authors.

Digital Object Identifier 10.1109/JSTARS.2021.3128355

[37], [38] ($1.3 \text{ km} \times 2.25 \text{ km}$) features a much smaller spatial resolution to compare and validate the EC tower-based GPP with satellite-derived SIF measurements. Besides, Chinese Carbon Dioxide Observation Satellite Mission (TanSat), launched on December 21, 2016, also provides unprecedented prospects in comparing satellite-based SIF with ground-based GPP measurements at the ecosystem scale with a significantly comparable spatial resolution ($2 \text{ km} \times 2 \text{ km}$) [39], [40]. Numerous studies have investigated the relationships between OCO-2 SIF and EC GPP measurements [41]–[43], whereas there are rarely relative studies on TanSat SIF products. The mismatched resolution between EC flux and space SIF is still the key problem in conducting research GPP with SIF. However, only OCO-2 SIF has comparable resolution with EC flux towers currently. In this context, TanSat SIF observations opened up a new perspective on investigating the mechanism link between satellite-based SIF and EC flux GPP measurements benefiting from the consistency of footprint size with flux towers. Furthermore, investigating the relationships between TanSat SIF and EC GPP will be useful for monitoring vegetation photosynthetic activity and carbon cycling at large scales by incorporating other satellite SIF products.

TanSat is the first Chinese satellite dedicated to accurately estimating carbon dioxide (CO_2) concentration at regional to continental scales. The high spectral resolution ($\sim 0.044 \text{ nm}$) at the $\text{O}_2\text{-A}$ band makes it possible to retrieve SIF products [44]. TanSat strategized three modes of observations—nadir, glint, and target modes—and a revisit period of 16 days. However, because of the strong Doppler shifts in the glint mode and the rarely small number of observations in the target mode, successful retrievals of SIF have only been conducted in the nadir modes. As a result, the TanSat SIF products covering the period from March 2017 to October 2019 for nadir mode have been obtained [39]. Nevertheless, TanSat has not been successfully operated since November 2019 due to the error of the satellite module.

In this article, we present the first investigation of the performance of the TanSat SIF dataset on GPP estimation using observations on various terrestrial vegetation biomes and assess how this relationship varied with different vegetation biomes. We collected EC flux observations of 203 flux sites and identified an EC dataset of 129 sites with concurrent TanSat coverage. First, we examined the relationships between TanSat SIF and EC GPP at Fe and KI bands for instantaneous and daily timescales. Second, we compared the correlations between EC GPP and TanSat SIF with moderate resolution imaging spectroradiometer (MODIS)-derived bidirectional reflectance distribution function (BRDF)-corrected VIs, including NDVI, EVI, and near-infrared reflectance of vegetation (NIR_v). Third, to further investigate the link between SIF and GPP, we evaluated the responses of SIF and GPP to photosynthetically active radiation (PAR), absorbed PAR (APAR), the fraction of APAR (FAPAR), and the product of APAR and two environmental factors, i.e., fT_{min} and $fVPD$. Finally, the performances of estimated GPP based on SIF, VIs, and light use efficiency (LUE) MODIS GPP algorithm were compared.

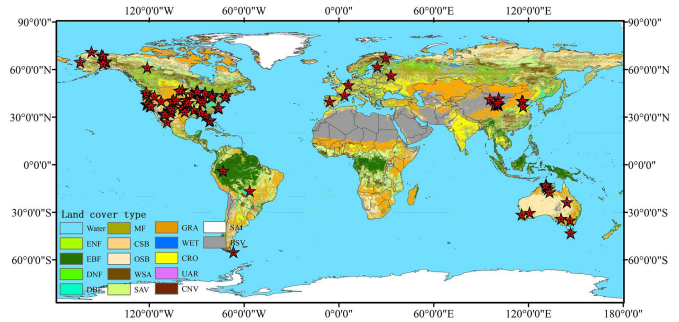


Fig. 1. EC flux site distribution. The land cover map is derived from the MODIS land cover type product (MCD12Q1) based on International Geosphere–Biosphere Programme (IGBP) classification scheme. CRO = the cropland type, GRA = grasslands type, DBF = deciduous broadleaf forests, ENF = evergreen needleleaf forests type, OSH = open shrublands type, SAV = savannas type, WSA = woody savannas type, MF = mixed forests type, WET = wetlands type, and BSV = bare or sparsely vegetated type.

II. MATERIALS AND METHODS

A. Site Descriptions

A total of 203 EC flux sites across the globe were screened to match the synchronous observations of TanSat and flux tower measurements from March 2017 to October 2019. For each site, a search range of $\sim 5 \text{ km} \times 5 \text{ km}$ was exploited to search the observations that TanSat overpasses the EC flux towers. TanSat operates a revisit period of 16 days and it cannot acquire the global continuous imager, which results in highly limited daily coverages especially under a single observation mode. Consequently, the availability of synchronous observations of TanSat surrounding flux sites within 5 km was largely constrained. There were no TanSat overpasses within the search range of 5 km surrounding the flux tower for part of EC flux sites. For some EC flux sites, there were one or few more observations of TanSat overpasses; meanwhile, on the one hand, concurrent flux measurements were observed or shared, on the other hand, no successfully retrieved SIF signals were obtained due to the quality of TanSat spectrum measurements. Besides, some highly heterogeneous flux sites were excluded according to the MODIS land cover data. Ultimately, 129 EC flux sites were selected, which included both flux measurements and TanSat SIF retrievals, and a number range from 1 to 7 of successfully retrieved SIF footprints of TanSat encompassing each flux site was identified. Fig. 1 depicts the 129 selected EC flux site distribution having TanSat SIF overpasses. Nine major vegetation biome types were encompassed by the selected flux sites: 14 cropland (CRO), 31 grassland (GRA), 15 deciduous broadleaf forest (DBF), 27 evergreen needle leaf forest (ENF), 8 open shrubland (OSH), 9 savanna (SAV), 7 woody savanna (WSA), 9 mixed forest (MF), and 9 wetlands (WET) sites. Detailed information, including the site ID, name, latitude, longitude, biome type, and the number of TanSat SIF overpasses are summarized in Table SI in Supplementary Material. The average time of successfully retrieved TanSat SIF encompassing each site was ~ 2.3 from March 2017 to October 2019.

B. EC Flux Data

EC systems, comprising a 3-D sonic anemometer to measure 3-D velocity and temperature and an open path infrared CO₂/H₂O gas analyzer to measure CO₂ and H₂O density, and an automatic weather station were used to measure the flux exchange between the ecosystem and atmosphere, as well as meteorological variables for each EC flux site [45]. Raw EC data with a 10-Hz sampling frequency were postprocessed to high-quality flux data with a 30-min interval after data filtering using EddyPro software [46]–[48]. Online tools available on the Max Planck Institute for Biogeochemistry's website¹ were exploited to calculate GPP after conducting the gap-filling and flux partitioning processes. In these processes, GPP data based on nighttime and daytime partitioning [49], [50] approaches were calculated. However, GPP data based on the nighttime approach were not successfully calculated for some sites due to the poor quality of vapor pressure deficit and temperature measurements. A previous study has demonstrated that the difference in GPP estimations using 23 different flux partitioning methods was less than 10% [51]. Therefore, to make exploit the EC flux dataset, GPP estimation based on daytime partitioning algorithm was used in this study.

C. TanSat SIF Data

TanSat SIF product was employed to investigate the relationship between satellite-derived SIF and EC GPP data. TanSat SIF data were retrieved using level 1B radiance data of O₂-A band derived by Atmospheric Carbon dioxide Grating Spectrometer (ACGS) maintained at the National Satellite Meteorological Center, China Meteorological Administration [39]. Two far-red SIF data at 758 and 771 nm (hereinafter, SIF_{Fe} and SIF_{KI}, respectively) retrieved using a data-driven algorithm accompanied by an auxiliary geometrical dataset were included in the SIF product. In addition, owing to the poor quality of spectrum measurements of O₂-A band in the glint mode, only SIF data in the nadir mode were successfully retrieved. Besides the instantaneous values of SIF at ~13:30 local time, daily SIF values could also be available making use of the daily mean factor calculated based on the strong correlation between PAR and solar zenith angle [38], [39]. Furthermore, the daily correction factors were provided in the public TanSat SIF dataset [39]. Eventually, to maintain the available amount of TanSat SIF soundings surrounding EC sites and decrease the influence of heterogeneous land surface of EC sites, TanSat SIF soundings were extracted within 5 km from each flux tower. Owing to the smaller spatial resolution of 2 km for TanSat, TanSat SIF soundings with the same land cover type for each site within 5 km were finally selected and directly averaged, which was to maintain consistency between TanSat SIF soundings and flux sites. On the one hand, most EC sites are homogeneous at the limited spatial scales of hundreds of meters or a few kilometers, which depends on the height of EC towers. On the other hand, the highly heterogeneous flux sites were rejected in this article.

¹[Online]. Available: <https://www.bgcjena.mpg.de/bgi/index.php/Services/REddyProcWeb>

D. MODIS Products

Three MODIS-derived satellite products with a 500-m spatial resolution were employed in this study; they were obtained from the NASA Level-1 and Atmosphere Archive and Distribution System Distributed Active Archive Center (LAADS DAAC). To distinguish the heterogeneities around available sites, the MODIS land cover product (MCD12Q1) and IGBP classification scheme were used as criteria for discrimination. Two MODIS reflectance products, including daily nadir BRDF-adjusted reflectance product, MCD43A4, and Aqua reflectance product, MYD09GA, were used to derive NDVI, EVI, and NIR_v for comparisons. A 4-day composite FPAR dataset, MCD15A3H, was also used to calculate the tower-based APAR based on flux PAR measurements for further comparisons with SIF and GPP.

E. Statistical Analysis

First, we evaluated the relationship of TanSat SIF and EC GPP at both Fe and KI bands for instantaneous and daily timescales using the 129 EC site observations. Almost all EC flux sites had half-hourly GPP data, whereas two sites (US-MMS and US-Ne1) only provided hourly GPP data. To match the equator crossing time of TanSat, the instantaneous GPP data were extracted from the half-hourly averaged values from 1:00 to 1:30 P.M. for almost all sites and the hourly data were interpolated to obtain the midday instantaneous GPP observations for the sites. Meanwhile, three VIs, MODIS-derived NDVI, EVI, and NIR_v, were compared with EC GPP and TanSat SIF. The VIs were calculated from two MODIS-derived reflectance products for the days having TanSat SIF. In addition, to investigate whether the SIF–GPP relationships differed across vegetation biomes, which had been reported in previous studies [9], [21], [52], the selected global EC measurements were separately used to fit the SIF–GPP relationship for each biome and the differences in the slopes of the SIF–GPP relationships were examined. As for the selection of EC sites, two steps were conducted on determining whether a site should be retained or rejected. First, a site that had concurrent TanSat SIF soundings and GPP observations could be retained. Second, Shannon's Diversity Index (SHDI, less than 2.10), calculated based on the IGBP land cover product of MCD12Q1 dataset, was used to determine whether a site should be retained or rejected. Then, we analyzed the relationships between SIF at Fe band, EC GPP and PAR, FAPAR, APAR. Furthermore, two environmental factors, i.e., *fTmin* and *fVPD*, used in MODIS GPP estimations based on the LUE model were multiplied by APAR for comparison with TanSat SIF and EC GPP. Two environmental factors were derived from the meteorological observations.

Finally, to investigate whether SIF had advantages on GPP estimations, the GPP estimate from TanSat SIF was comparable to those from MODIS EVI, NIR_v, and EC GPP and LUE-based MODIS GPP algorithm using all the concurrent TanSat SIF and EC site observations for all biomes. For SIF and VIs methods, *K*-fold cross-validation was carried out to assess the performances of estimating GPP. Considering the amount of the dataset, we set *K* as 10 in this study, i.e., the fitting processes were all performed

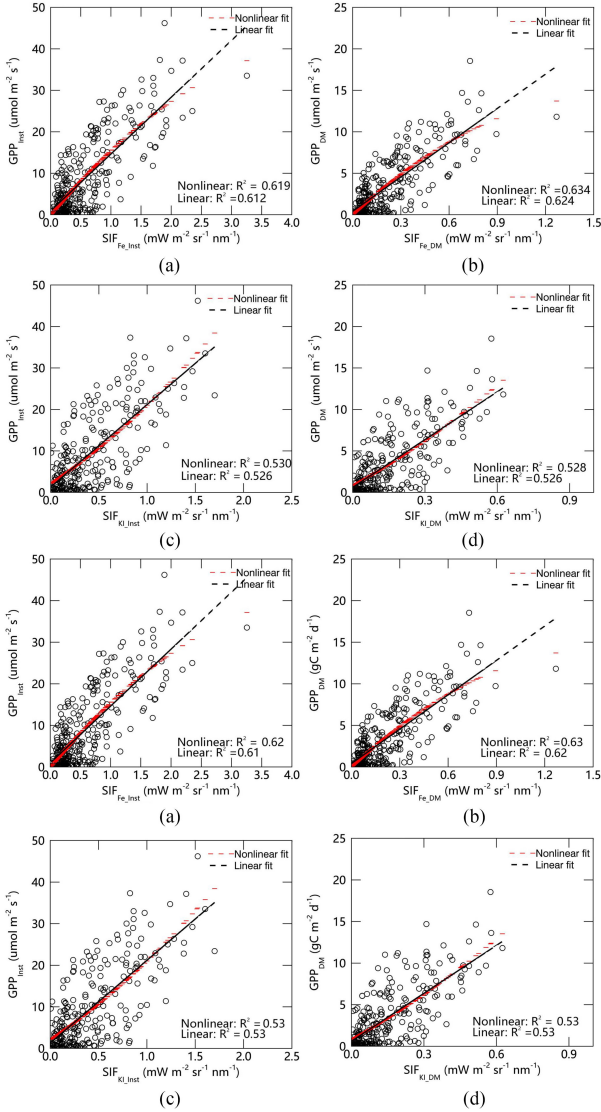


Fig. 2. Relationships between (a) and (b) TanSat SIF and EC GPP at Fe and (c) and (d) KI bands for instantaneous (a) and (b) and daily (b) and (d) timescales.

10 times; then, the averaged fitted GPP was regarded as the final fitted GPP to compare with true EC GPP values. We employed the coefficient of determination (R^2) and root-mean-square error (RMSE) to evaluate their predictive abilities.

III. RESULTS

A. Comparisons Between TanSat SIF and VIs With EC GPP

As shown in Fig. 2, strong linear relationships between TanSat SIF and flux tower GPP were observed at Fe and KI bands regardless of the timescale, which showed that the correlations between TanSat SIF and GPP were better at Fe band ($R^2 = 0.61$ for SIF_{Inst} and $R^2 = 0.62$ for SIF_{DM}) than at KI band ($R^2 = 0.53$ for SIF_{Inst} and $R^2 = 0.53$ for SIF_{DM}) for both timescales. Meanwhile, no obvious advantages of goodness-of-fit for daily scale compared with that for instantaneous scale was observed, especially for KI band. Moreover, it can be found that the accuracy of nonlinear

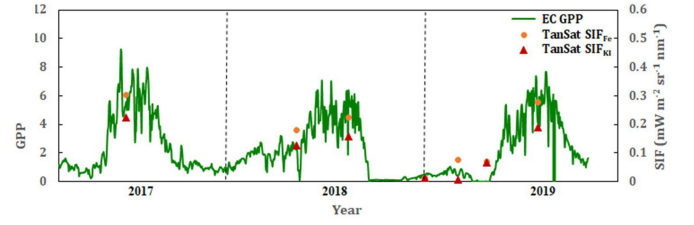


Fig. 3. Seasonal trajectories of GPP and daily TanSat SIF at an EC grassland site (CN-SDQ) from March 1, 2017, to October 31, 2019.

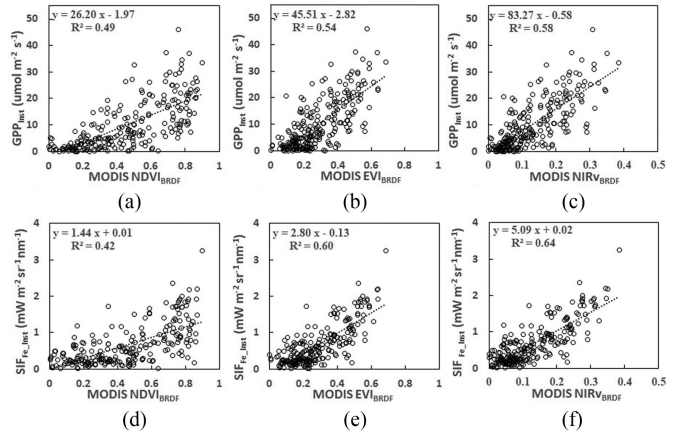


Fig. 4. Relationships between MODIS BRDF-corrected NDVI, EVI, and NIR_v derived from MCD43A4 reflectance product with (a)–(c) EC GPP and (d)–(f) TanSat SIF, respectively.

(hyperbolic) models had no obvious differences compared with that of a linear model for both bands and timescales.

Fig. 3 illustrated the seasonal trajectories of EC GPP and TanSat SIF at Sidaoqiao (CN-SDQ) site, which has a relative frequent visit with seven valid soundings. CN-SDQ site is located along the lower reaches of the Heihe hydrometeorological observation network in Sidao Bridge, Ejina Banner, Inner Mongolia, China (101.14° E, 42.00° N). Although the amount of available concurrent TanSat SIF and EC GPP samples was very limited, they covered different grassland growing period of site CN-SDQ except for the late growing stage. We found that TanSat-derived SIF at both Fe and KI band well tracked the seasonal cycle of EC GPP, which indicates the potential of satellite-derived SIF on estimating GPP.

To help assess the feasibility of TanSat SIF for estimating GPP, further comparisons between three VIs, NDVI, EVI, and NIR_v , derived from MODIS BRDF-corrected reflectance products with EC GPP and TanSat SIF at Fe band were first examined (see Fig. 4). Overall, strong relationships between VIs and EC GPP were observed with values of R^2 ranging from 0.49 to 0.58. NIR_v performed best on interpreting GPP, whereas NDVI showed the weakest correlation with EC GPP among three VIs. Nevertheless, the relationship between NIR_v and EC GPP ($R^2 = 0.58$) was still weaker than that between TanSat SIF and EC GPP ($R^2 = 0.61$). We also compared VIs with TanSat SIF at Fe band in Fig. 4. Similarly, NIR_v ($R^2 = 0.64$) had the strongest correlation with SIF than EVI ($R^2 = 0.60$) and NDVI ($R^2 = 0.42$). In addition, EVI and NIR_v showed much stronger correlations with

SIF than with GPP. Owing to the NDVI saturation at high values, the correlations between NDVI with GPP and SIF were discrete. Therefore, EVI and NIR_v correlated more with GPP or SIF than NDVI. Meanwhile, to make a strict analysis on matching TanSat SIF and MODIS VIs according to the overpassing time of TanSat, we also compared these three VIs derived from Aqua MODIS reflectance product (MYD09GA) with EC GPP and TanSat SIF, as illustrated in Fig. S1. The results showed that EC GPP or TanSat SIF exhibited much stronger correlations with VIs derived from the BRDF-corrected reflectance than that based on Aqua product. This indicated that the varying observation geometry could strongly affect the reflectance of an object on the Earth, which will also affect the reflectance-derived VIs, especially for NDVI.

B. Relationships Between TanSat SIF and GPP With APAR

To further investigate the link between TanSat SIF and EC GPP, we assessed the relationships between SIF and GPP with PAR, FAPAR, APAR, and $APAR \times fT_{min} \times fVPD$ (see Fig. 5). It showed that PAR, FAPAR, and APAR explained 13%, 45%, and 59% of the variance in SIF at Fe band and 11%, 53%, and 60% of the variance in EC GPP. Discrete scatters were found between SIF, GPP, and PAR. APAR, the product of PAR and FAPAR, explained much more variance in both SIF and GPP than PAR or FAPAR alone. In addition, the correlations between pairs of SIF, GPP, and APAR tended to linearize and converge, which indicated that SIF and GPP mainly depend on APAR, resulting in the strong link between SIF and GPP. Furthermore, the product of APAR and environmental scaling factors derived from two simultaneous meteorological measurements was employed for comparisons with TanSat SIF and EC GPP. As shown in Fig. 5, except for APAR, other environmental factors will also influence SIF and GPP. However, GPP was much more influenced by environmental factors than SIF, attributable to the effects of environmental factors on photosynthetic LUE (LUE_p).

To make further comparisons between VIs and SIF on mechanism links with GPP, the relationships between EVI and NIR_v with FAPAR, APAR, and $APAR \times fT_{min} \times fVPD$ are also illustrated in Fig. 6 to investigate whether VIs could explain physiological information of GPP except for structural information. NIR_v and EVI showed strong correlations with FAPAR, APAR, and $APAR \times fT_{min} \times fVPD$. The relationships of the VIs with FAPAR were much stronger than those with APAR, with the highest values of R^2 as 0.73 and 0.74 for EVI and NIR_v , respectively. The relationships strengthened when considering the impact of environmental factors but were still weaker than that with FAPAR, which revealed that EVI and NIR_v mainly contained information on FAPAR and partly accounted for environmental effects.

C. Biome-Specific Relationships Between TanSat SIF and EC GPP

To investigate whether a unique relationship exists between satellite-based SIF and EC GPP across different biomes, we examined the relationships between EC GPP and TanSat SIF at both bands and timescales for nine biomes (see Figs. 7 and 8).

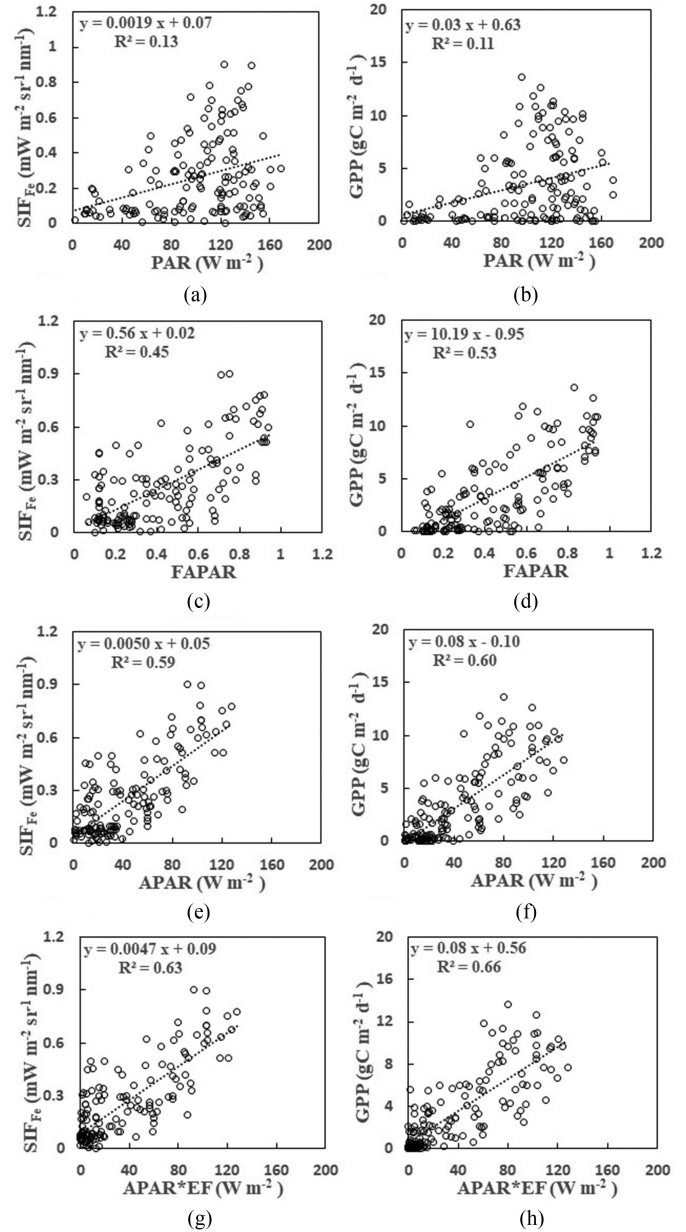


Fig. 5. Relationships between TanSat SIF and GPP with PAR, FAPAR, APAR, and $APAR \times EF$. EF is the product of fT_{min} and $fVPD$. SIF at Fe band versus (a) PAR, (c) FAPAR, (e) APAR, and (g) $APAR \times EF$. EC GPP versus (b) PAR, (d) FAPAR, (f) APAR, and (h) $APAR \times EF$.

They showed that overall linear correlations between TanSat SIF and EC GPP were found for all nine biomes. For the Fe band, consistently significant relationships between SIF and GPP were observed with R^2 greater than 0.44 at both instantaneous and daily timescales for all biomes except OSH whose R^2 was only 0.11 and 0.17 at instantaneous timescale and daily timescale, respectively. Similarly, the weakest relationships were also found for the OSH biome at the KI band at both instantaneous ($R^2 = 0.18$) and daily ($R^2 = 0.25$) timescales. Further comparison between different timescales showed that for relationships between EC GPP and TanSat SIF at the Fe band for instantaneous timescale, overall weaker goodnesses-of-fit ($R^2 = 0.11$ – 0.81)

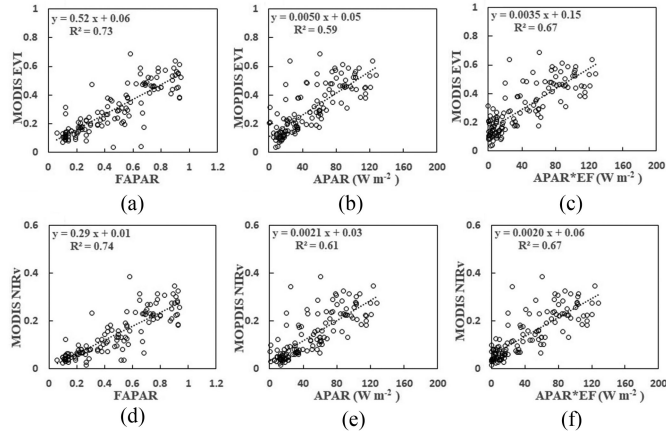


Fig. 6. Relationships between MODIS VIs with FAPAR, APAR, and APAR \times EF. EF is the product of fT_{min} and $fVPD$. EVI versus (a) FAPAR, (b) APAR, and (c) APAR \times EF. NIR $_v$ versus (d) FAPAR, (e) APAR, and (f) APAR \times EF.

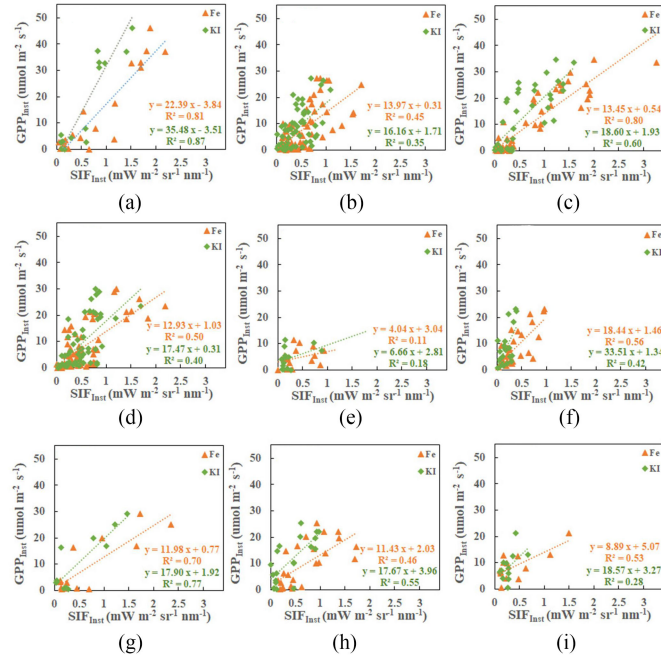


Fig. 7. Relationships between TanSat SIF and EC GPP for nine biomes at both Fe and KI bands for instantaneous timescale. (a) CRO = the cropland type. (b) GRA = grasslands type. (c) DBF = deciduous broadleaf forests. (d) ENF = evergreen needleleaf forests type. (e) OSH = open shrublands type. (f) SAV = savannas type. (g) MF = mixed forests type. (h) WET = wetlands type. (i) WSA = woody savannas type.

were observed than those of daily timescale ($R^2 = 0.17\text{--}0.86$) for all nine biomes. In addition, the differences in goodness-of-fit were even smaller at the KI band with values of R^2 in the range of 0.18–0.87 and 0.25–0.85 for instantaneous and daily timescales, respectively.

As illustrated in Figs. 7 and 8, the slopes of line relationships were greatest for CRO at Fe band (22.39 $\mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}/\text{mW}\cdot\text{m}^{-2}\cdot\text{sr}^{-1}\cdot\text{nm}^{-1}$ and 20.56 $\text{gC}\cdot\text{m}^{-2}\cdot\text{d}^{-1}/\text{mW}\cdot\text{m}^{-2}\cdot\text{sr}^{-1}\cdot\text{nm}^{-1}$ for instantaneous and daily timescales, respectively) and KI band (35.48 $\mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}/$

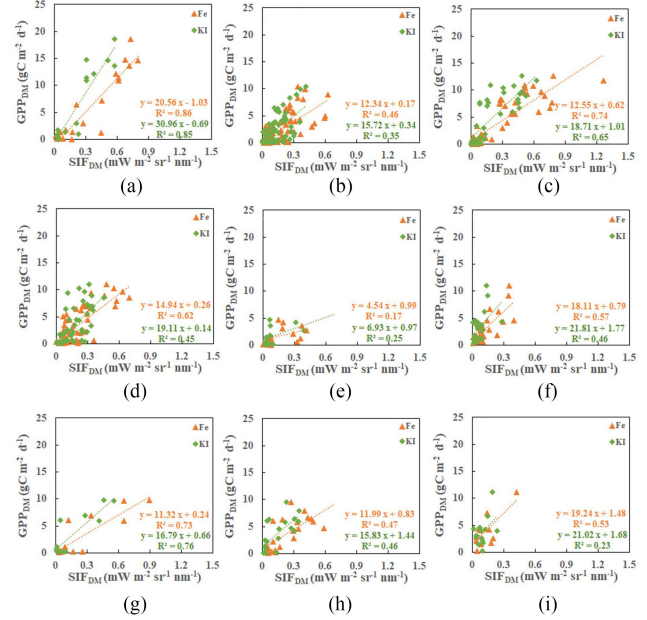


Fig. 8. Relationships between TanSat SIF and EC GPP for nine biomes at both Fe and KI bands for daily timescale. (a) CRO = the cropland type. (b) GRA = grasslands type. (c) DBF = deciduous broadleaf forests. (d) ENF = evergreen needleleaf forests type. (e) OSH = open shrublands type. (f) SAV = savannas type. (g) MF = mixed forests type. (h) WET = wetlands type. (i) WSA = woody savannas type.

$\text{mW}\cdot\text{m}^{-2}\cdot\text{sr}^{-1}\cdot\text{nm}^{-1}$ and 30.96 $\text{gC}\cdot\text{m}^{-2}\cdot\text{d}^{-1}/\text{mW}\cdot\text{m}^{-2}\cdot\text{sr}^{-1}\cdot\text{nm}^{-1}$ for instantaneous and daily timescales, respectively) and smallest for OSH with values of the slope of 4.04 $\mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}/\text{mW}\cdot\text{m}^{-2}\cdot\text{sr}^{-1}\cdot\text{nm}^{-1}$ and 4.54 $\text{gC}\cdot\text{m}^{-2}\cdot\text{d}^{-1}/\text{mW}\cdot\text{m}^{-2}\cdot\text{sr}^{-1}\cdot\text{nm}^{-1}$ for the Fe band and 6.66 $\mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}/\text{mW}\cdot\text{m}^{-2}\cdot\text{sr}^{-1}\cdot\text{nm}^{-1}$ and 16.93 $\text{gC}\cdot\text{m}^{-2}\cdot\text{d}^{-1}/\text{mW}\cdot\text{m}^{-2}\cdot\text{sr}^{-1}\cdot\text{nm}^{-1}$ for the KI band. At Fe and KI bands, the remaining biomes, except for SAV, had relatively similar slopes at instantaneous and daily timescales, respectively. The differences in slopes of the SIF–GPP relationships for all biomes were much smaller at both timescales for the Fe band than for the KI band; only the relationships for CRO and OSH were significantly different from other biomes for the KI band at both timescales. In general, the slopes of the SIF–GPP relationships were slightly larger at instantaneous timescale than at daily timescale for both bands.

A high correlation between biome-averaged GPP and averaged SIF across nine biomes was observed, as shown in Fig. 9. Similar to the results of Fig. 2, the SIF–GPP relationship at daily time scale ($R^2 = 0.76$ and 0.65 at Fe and KI bands, respectively) was stronger than at instantaneous timescale ($R^2 = 0.73$ and 0.63 at Fe and KI bands, respectively). In addition, Fig. 9 shows the remarkable advantages of SIF at Fe band on GPP estimation across biomes.

D. Evaluating the Performance of Satellite SIF on Estimating GPP

The performance of satellite-based SIF on estimating GPP using the SIF–GPP relationship derived from TanSat SIF at the

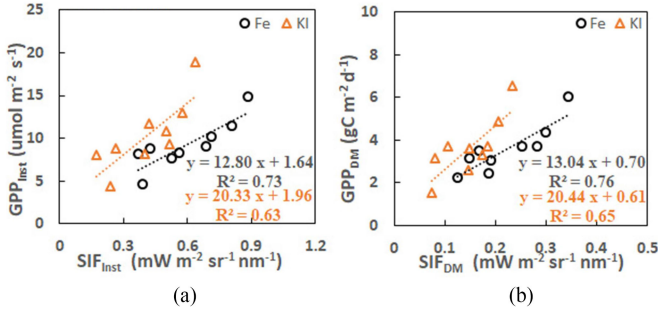


Fig. 9. Scatter plot of biome-averaged TanSat SIF and EC GPP data for nine biomes at Fe and KI bands for (a) Instantaneous and (b) Daily timescales.

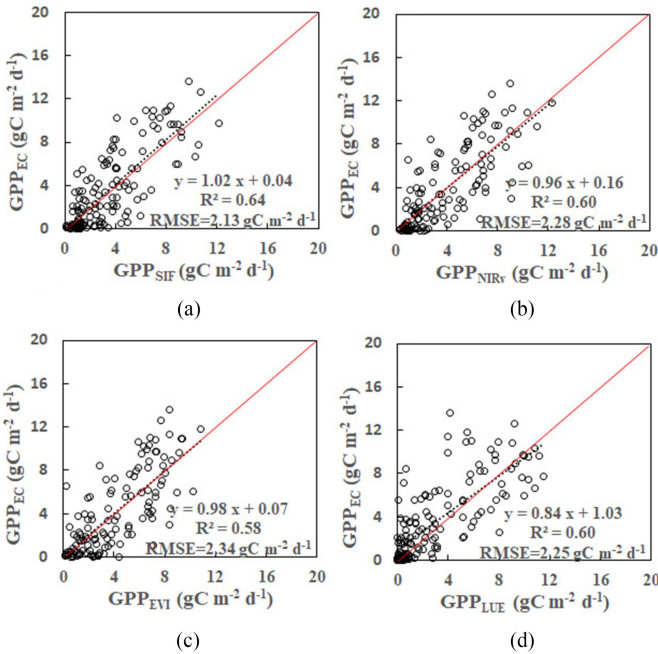


Fig. 10. Comparisons between EC GPP and estimated GPP derived from linear relationships between EC GPP and (a) TanSat SIF. (b) MODIS NIR_v. (c) EVI. and (d) LUE model (MODIS GPP algorithm).

Fe band and EC GPP for different biomes was evaluated using a ten-fold cross-validation approach. Considering the availability of auxiliary data used in the LUE model and the consistency of datasets used for four models, the validation dataset used was slightly less than that in Fig. 2. The overall good correspondence between EC GPP and GPP estimates could be observed (see Fig. 10). From Fig. 10(a), the SIF-based GPP estimates derived from TanSat data at the Fe band had a good linear relationship with EC GPP ($R^2 = 0.64$, $RMSE = 2.13 \text{ gC}\cdot\text{m}^{-2}\cdot\text{d}^{-1}$) with all the points lying near the 1:1 line, indicating a high degree of consistency between them. Besides the SIF-based GPP estimates, we also performed GPP estimation using a VI-based algorithm and the traditional LUE-based model (MODIS GPP algorithm). The GPP estimates based on NIR_v had comparable performances to the MODIS GPP algorithm with R^2 of both as 0.60 and RMSE of 2.28 and 2.25 $\text{gC}\cdot\text{m}^{-2}\cdot\text{d}^{-1}$ for NIR_v and MODIS GPP algorithm, respectively. However, the scatter plots of the relationship between EC GPP and GPP estimates

based on the MODIS GPP algorithm were more discrete. EVI performed slightly worse than NIR_v and MODIS algorithm as well as SIF with R^2 of 0.58 and the highest RMSE of 2.34 $\text{gC}\cdot\text{m}^{-2}\cdot\text{d}^{-1}$. In general, VI-based and MODIS GPP algorithms slightly underestimated GPP, especially at high values of GPP. Overall, the results showed that satellite-based SIF could be used for GPP estimation slightly better than VI-based and MODIS GPP algorithm.

IV. DISCUSSION

Previous studies have demonstrated significant relationships between GOME-2 or GOSAT SIF and gridded GPP [9], [11], [21], [52]. However, owing to the uncertainties of gridded GPP and coarse spatial resolutions of GOME-2 and GOSAT, direct comparison between GOSAT and GOME-2 SIF products with EC flux GPP has been hindered. In general, the spatial scale mismatch was a key difficulty in validating or comparing satellite-based remote sensing products with ground observations. Afterward, OCO-2 provided the first opportunity for evaluating the relationship between satellite SIF and EC flux GPP observations due to its fine spatial resolution of 1.3 km × 2.25 km [37]. In addition, several studies have employed OCO-2 SIF to investigate the relationship with flux tower GPP and found strong correlations between them [41], [42]. Similarly, it is possible to evaluate TanSat SIF using EC flux GPP with a 2-km spatial resolution. Such fine spatial resolution has advantages in matching satellites with tower footprint and conducting a site-scale analysis for satellite SIF with tower GPP.

Our results showed that strong correlations between TanSat SIF and EC GPP were observed at the Fe and KI bands for instantaneous and daily timescales. In addition, the relationship of GPP with SIF_{Fe} was much stronger than SIF_{KI}, whereas no significant distinctions on the relationship for instantaneous and daily timescales were observed. Previous works have found the stronger ability of SIF_{Fe} on estimating GPP than that of SIF_{KI} [41], [42], which was attributed to the much stronger signal of SIF_{Fe} than SIF_{KI}. In general, the signals of SIF_{Fe} was 1.4–1.7 times higher than that of SIF_{KI} [38]. On the one hand, SIF_{Fe} is closer to the far-red peak of SIF spectrum; on the other hand, the depth of Fraunhofer line at Fe band was much deeper than that at KI band, resulting more uncertainties in SIF retrievals at KI band than that at Fe band. Extensive previous studies have investigated the relationships between SIF and GPP. Generally, most studies reported linear relationships between SIF and GPP based on simulated datasets [53], [54], ground measurements [16], and satellite-based observations [9], [11], [21], [55]. By contrast, some studies also demonstrated that the nonlinear relationships existed between SIF and GPP at the instantaneous timescale or leaf scale [17], [19], and the relationships would be linear when SIF and GPP were at the canopy level or aggregated to daily timescale or other longer timescales. However, our global analysis showed obvious linear relationships between TanSat SIF and EC GPP even at an instantaneous timescale. Except for daily timescale, the differences in accuracy between linear and nonlinear models were even negligible at instantaneous timescale, which was seemingly contradictory with the previous

conclusions [17], [19]. This may result from the limited available satellite-based data soundings that matched with EC observations. In fact, the mechanistic and complex relationship between satellite SIF and EC GPP would be affected by many factors, such as light conditions, canopy or leaf structures, physiological responses, scale effects, and environmental factors [56], [57]. Therefore, how linear or nonlinear relationships are presented need more available measurements covering different temporal and spatial scales and further investigation in the future work.

Strong relationships between TanSat SIF and EC GPP were observed in eight of the nine biomes at both bands. The weakest relationships occurred in the OSH with R^2 ranging from 0.11 to 0.25. No significant differences in slopes of relationships between TanSat SIF and EC GPP were found, except for CRO and OSH biomes, especially for the Fe band, which was seemingly contradictory with previous works showing that the relationships between satellite SIF and GPP depended on vegetation biomes [21], [22], [31], [52], [58]. However, the biome-dependent SIF-GPP relationships may be slightly larger for the KI band. In fact, the biome-specific findings of the SIF-GPP relationships were mostly concluded from either GOME-2 SIF with coarse-spatial resolution or gridded GPP estimates with large estimated uncertainties. Previous studies have also found similar relationships between satellite SIF and GPP using OCO-2 SIF and individual or amount of EC flux GPP observations [23], [41]. Sun *et al.* found that crops, forest, and grass had similar slopes using limited concurrent observations (~ 30 samples) of OCO-2 SIF and EC tower GPP [23]. Similarly, Li *et al.* also observed similar slopes in SIF-GPP relationship using OCO-2 SIF₇₅₇ and tower GPP based on 64 sites, and the smallest slope was observed in EBF [41]. However, our results showed that the value of slope in CRO was much larger than forest biome and the weakest relationship and smallest slope were occurred in OSH. These could largely result from the differences in available concurrent satellite dataset used in comparison with EC GPP and the spatial heterogeneity in different EC sites. In our results, the uncertainties of OSH may result from the very limited number of TanSat observations (less than 20 samples) overpassing EC flux site for OSH biome with EC GPP ranging from 0 to $11.3 \mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$ at instantaneous timescale and from 0.04 to $4.65 \text{gC}\cdot\text{m}^{-2}\cdot\text{d}^{-1}$ for daily timescale for the matched samples. Therefore, the slopes and relationships for OSH may be altered if more valid matched samples are available. As for CRO, previous works have demonstrated that the canopy structure has a strong impact on the SIF-GPP relationship in crops [19], [20]. Moreover, photosynthetic pathways will affect the slopes of the SIF-GPP relationship. Liu *et al.* [54] reported that C_4 crops had a higher slope than C_3 type based on ground measurements. Therefore, the differences in slopes of SIF-GPP relationship for CRO require further studies.

To help evaluate the capability of TanSat SIF on estimating GPP, we examined the relationships between EC GPP and MODIS-derived NDVI, EVI, and NIR_v. Previous works have shown that satellite SIF correlated more with nadir BRDF-adjusted VIs than that derived from Terra or Aqua reflectance due to the effects of varying observation geometry on reflectance [41]. So, VIs calculated from MODIS BRDF-corrected

reflectance were used for comparisons, and we found stronger relationships between EVI, NIR_v, and EC GPP than NDVI but still slightly weaker than that for TanSat SIF. The result agreed with previous results, showing that SIF could better characterize the actual photosynthesis than traditional VIs [4]–[6]. The examination of the relationships between EVI or NIR_v and FAPAR showed their relationships were also better than that of EVI, NIR_v, and SIF or GPP, demonstrating that traditional VIs were great proxies for FAPAR, especially for EVI and NIR_v. Unlike VIs, SIF could account for information on instantaneous illumination, leading to sensitivity to rapid changes in physiology [15]. However, NIR_v presented similarly strong relationships with EC GPP and TanSat SIF, indicating that BRDF-corrected NIR_v derived from MODIS also have strong predictive ability for estimating GPP, consistent with that NIR_v could be regarded as a direct index of photons intercepted by chlorophyll [59]. Moreover, we observed the saturation phenomenon of relationships between SIF or GPP and NDVI, which contributes to the saturation of NDVI at high LAI [62]. So, EVI and NIR_v largely eliminated this disadvantage for dense vegetation. Meanwhile, the MODIS-derived NIR_v could be easily available and even more spatially and temporally continuous compared to SIF [59]–[61]. From this perspective, NIR_v could also be used for estimates of GPP at site level or global scale and has unique advantages on data amount.

To further reveal the mechanisms underlying the SIF-GPP relationship, we investigated how SIF and EC GPP responded to APAR, respectively. Many previous studies suggested that the SIF-GPP relationship was dominated by APAR [63], whereas a recent study highlighted the dominant role of canopy structure in the SIF-GPP relationship for CRO biome [20]. Our results showed much higher correlations between TanSat SIF, EC GPP, and APAR compared to PAR. Moreover, except for APAR, we found that SIF responded to environmental factors (fTmin and fVPD) similar to GPP. The correlations between the products of these two environmental factors and APAR explained more variances of TanSat SIF and EC GPP than APAR alone. Several previous works also identified environmental control factors influencing both SIF and GPP using GOME-2 and OCO-2 SIF observations [41], [64]. Low air temperature and VPD could regulate photosynthesis ability by affecting the effective maximum rate of carboxylation and stomatal conductance and intercellular CO₂ concentration, respectively, which result in LUE_p variation. The results of this study showed that the LUE_p determination could also influence SIF, which indicated the mechanism foundation of the application of SIF on estimating GPP. However, how SIF_{yield} or f_{esc} respond to LUE_p requires further investigation.

Our comparisons of estimated GPP based on the SIF and LUE model showed the predictive ability of SIF was slightly better than the MODIS GPP algorithm. A series of ancillary variables, including PAR and FAPAR, and different environmental factors, as well as biome classification products, were required in the MODIS GPP algorithm. However, these variables used in the MODIS GPP model have significant uncertainties [65], which will lead to large uncertainties on GPP estimations. Moreover, previous works have demonstrated the underestimation of

MODIS GPP compared with EC GPP. Unlike the LUE model, the GPP estimated method based on SIF does not need the above ancillary dataset, which will reduce uncertainties in the GPP estimation of the LUE-based model. Meanwhile, SIF has excellent performance on estimating GPP, thus could potentially be widely used in further carbon cycling works.

Despite the great performance of SIF on estimating GPP, the wide application of TanSat SIF on regional or global GPP estimation is still challenging. First, it is extremely difficult to obtain long-term continuous and wide-spatial coverage of TanSat SIF due to the spatially and temporally sparse coverage of TanSat. On one hand, only TanSat SIF products at nadir mode were successfully retrieved due to the quality problem of data in the glint mode, which result in the reduction of approximately half of the TanSat data available. It was difficult to generate gridded SIF at high spatial and temporal resolutions. On the other hand, TanSat data have not been available since November 2019 due to the instrument breakdown. Second, the available number of EC flux data for most sites is limited and the public datasets also have significant uncertainties, especially for a missing problem. Therefore, only a few TanSat SIF observations were available for most EC flux sites over the globe in this study. It was impossible to conduct seasonal and even interannual analyses in vegetation photosynthesis or phenology at the site scale and examine the relationships over space. Further examinations of the relationship between TanSat SIF and EC GPP will need more available matched soundings for several vegetation biomes, such as OSH and SAV. One solution is to expect that more EC flux datasets could be public in the future. Another possible solution is to incorporate other spatially and temporally continuous satellite datasets, e.g., MODIS, GOME-2 and TROPOMI SIF products, with TanSat SIF to generate continuous SIF estimates based on machine learning algorithm [66].

V. CONCLUSION

We have used the nearly concurrent TanSat SIF and global EC flux observations (March 2017 to December 2019) encompassing 129 EC flux sites and covering 9 major vegetation biomes to analyze the relationship between satellite-based SIF and EC GPP at two bands (Fe and KI) for two timescales (instantaneous and daily). Significant relationships between TanSat SIF and EC GPP were observed at both Fe and KI bands for instantaneous and daily timescales with much stronger relationships at the Fe band than the KI band. EC GPP was more strongly correlated with TanSat SIF at Fe band ($R^2 = 0.61$) than MODIS-derived BRDF-corrected NDVI ($R^2 = 0.49$) and slightly better than with BRDF-corrected EVI ($R^2 = 0.54$) and NIR_v ($R^2 = 0.58$). We further investigated the responses of TanSat SIF and EC GPP to APAR and two environmental factors and found that SIF was dominated by APAR and also influenced by environmental factors similar to GPP. Strong correlations between TanSat SIF and EC GPP were shown for all biomes except for OSH ($R^2 = 0.11$ – 0.25), and a consistent relationship was observed across nine biomes except for CRO and OSH with much higher and lower slopes, respectively. The GPP estimates based on SIF performed better than those based on EVI and NIR_v as

well as the MODIS GPP algorithm. Therefore, TanSat provides an unprecedented SIF dataset comparable to ground-based EC measurements with fine spatial resolution. In addition, we demonstrated the predictive ability of TanSat SIF on estimating GPP. Combining TanSat SIF having fine spatial resolution with other satellite SIF products (e.g., GOME-2, TROPOMI, OCO-2, and FLEX) will be helpful for future carbon cycling studies.

ACKNOWLEDGMENT

The authors would like to acknowledge the AmeriFlux Network and National Tibetan Plateau Third Pole Environment Data Center for making the EC flux data public, and Prof. Shaomin Liu and Dr. Ziwei Xu at Beijing Normal University and Yongguang, Zhang for providing the flux datasets. The authors would also like to thank the MODIS data processing team for making available the MODIS data. All the MODIS data were obtained from the NASA Level-1 and Atmosphere Archive and Distribution System Distributed Active Archive Center (LAADS DAAC).

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