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Chlorophyll fluorescence observed by OCO-2 is strongly related to gross primary productivity estimated from flux towers in temperate forests

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ABSTRACT

Solar-induced chlorophyll fluorescence (SIF) opens a new perspective on the monitoring of vegetation photosynthesis from space, and has been recently used to estimate gross primary productivity (GPP). However, previous studies on SIF were mainly based on satellite observations from the Greenhouse Gases Observing Satellite (GOSAT) and Global Ozone Monitoring Experiment-2 (GOME-2), and the evaluation of these coarse-resolution SIF measurements using GPP derived from eddy covariance (EC) flux towers has been hindered by the scale mismatch between satellite and tower footprints. We use new far-red SIF observations from the Orbiting Carbon Observatory-2 (OCO-2) with much finer spatial resolution and GPP data from EC flux towers from 2014 to 2016 to examine the relationship between GPP and SIF for temperate forests. The OCO-2 SIF tracked tower GPP well, and had strong correlation with tower GPP at both retrieval bands (757 nm and 771 nm) and both instantaneous (mid-day) and daily timescales, with the strongest relationship for the 757 nm band (SIF757) at the daily timescale. Daily SIF757 exhibited much stronger correlation with tower GPP compared to the enhanced vegetation index (EVI) and normalized difference vegetation index (NDVI) based on the surface reflectance product derived from the moderate resolution imaging spectroradiometer (MODIS) onboard either Terra or Aqua satellite and had a similarly strong relationship as EVI based on the bidirectional reflectance distribution function (BRDF) corrected reflectance product (MCD43A4) based on data from both Terra and Aqua. Absorbed photosynthetically active radiation (APAR) explained 85% of the variance in SIF757, while the product of APAR and two environmental scalars - $f\Gamma_{min}$ and fVPD (representing minimum temperature stress and water stress) explained higher variance (92%) in SIF₇₅₇. This suggests that SIF mainly depends on APAR and is also affected by environmental stresses that determine photosynthetic light use efficiency. The BRDF-corrected EVI also has advantages over SIF in that EVI has spatially and temporally continuous coverage and has a much longer record (2000-present). The OCO-2 SIF₇₅₇ estimated GPP well ($R^2 = 0.81$, p < 0.0001; RMSE = 1.11 gC m⁻² d⁻¹), and its performance was comparable to or slightly better than that of the MODIS GPP algorithm, a GPP model based on the light use efficiency logic. With intensive OCO-2 observations acquired in the Target mode around Park Falls, a calibration/validation site for OCO-2, we also generated gridded SIF and then estimated GPP on a per-pixel basis at the landscape scale. Our findings demonstrate the strong ability of chlorophyll fluorescence observed by OCO-2 in estimating GPP for temperate forests and reveal its potential and limitations in future ecosystem functioning and carbon cycling studies.

1. Introduction

Terrestrial gross primary productivity (GPP), carbon fixation by terrestrial plants via photosynthesis, is the largest carbon flux between the terrestrial biosphere and the atmosphere. Terrestrial GPP dominates the interannual variability of the terrestrial ecosystem carbon uptake (Amiro et al., 2010; Schwalm et al., 2010; Xiao et al., 2009) and also drives the terrestrial food chain (Verma et al., 2017). Therefore,

accurate estimation of GPP is essential for assessing ecosystem functioning, carbon budgets, and food production in the context of global change (Duveiller and Cescatti, 2016; Grace et al., 2007; Houborg et al., 2013; Zhang et al., 2014).

Satellite remote sensing has been widely used to estimate GPP at various spatial and temporal scales. For example, the satellite-derived vegetation indices (e.g., normalized difference vegetation index, NDVI; enhanced vegetation index, EVI) and canopy biophysical variables (e.g.,

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chlorophyll content; leaf area index, LAI; the fraction absorbed photosynthetically active radiation by vegetation, fPAR) have been used to estimate GPP for a variety of ecosystem types (Gitelson et al., 2012; Peng and Gitelson, 2012; Running et al., 2004; Tucker and Sellers, 1986; Xiao et al., 2010; Zhang et al., 2009). The light use efficiency (LUE) logic (Monteith, 1972; Monteith and Moss, 1977) is perhaps the most widely used approach for estimating GPP from remotely sensed data. The LUE approach can be expressed as follows:

$$GPP = fPAR \times PAR \times LUE_p = APAR \times LUE_p \tag{1}$$

where PAR is photosynthetically active radiation, and LUE $_{\rm p}$ denotes photosynthetic light use efficiency, the efficiency at which absorbed radiation is used in the process of photosynthesis. This logic has been implemented in a number of LUE or process-based ecosystem models for estimating GPP, and fPAR is typically based on vegetation indices (Potter et al., 1993; Xiao et al., 2004) or the fPAR product derived from the moderate resolution imaging spectroradiometer (MODIS) (Running et al., 2004). However, vegetation indices such as NDVI and EVI are not sensitive to rapid changes in plant photosynthetic status resulting from physiological changes induced by environmental stresses (e.g., heat, water stress) (Dobrowski et al., 2005; Daumard et al., 2010; Zarco-Tejada et al., 2013; Rascher et al., 2015), while those changes can be captured by solar-induced chlorophyll fluorescence (SIF) (Daumard et al., 2010; Zarco-Tejada et al., 2013; Joiner et al., 2014; Rascher et al., 2015).

In the recent few years, SIF opens a new perspective on the monitoring of vegetation photosynthetic activity from space (Frankenberg et al., 2011; Guanter et al., 2012; Joiner et al., 2013; Joiner et al., 2011; Joiner et al., 2014). SIF is essentially a "glow" of plants under sunlight, and is an energy flux emitted from plant chlorophyll molecules a few nanoseconds after light absorption in the wavelength range from 600 to 800 nm (Baker, 2008). Light energy absorbed by the leaf chlorophyll molecules has three different pathways: photochemistry, non-photochemical quenching (NPO, i.e., heat dissipation), and a small fraction re-emitted as SIF (Baker, 2008). SIF and NPQ compete with photosynthesis for the use of the absorbed light. This closely coupled relationship enables SIF to provide a direct and quick diagnosis of the actual photosynthesis status of vegetation. Therefore, SIF is more physiologically based compared to the traditional vegetation indices such as NDVI and EVI (Meroni et al., 2009; Zarco-Tejada et al., 2013). SIF can be expressed in a similar way as the LUE approach for estimating GPP (Eq. (1)) (Yoshida et al., 2015):

$$SIF = fPAR \times PAR \times SIF_{yield} = APAR \times \Theta_f \times \Omega_c$$
 (2)

where SIF_{yield} is the emitted SIF per photon absorbed, which is the product of $\Theta_{\rm f}$ the fluorescence yield at the membrane scale, and $\Omega_{\rm c}$, a structural interference determining the fraction of SIF photons escaping the canopy. The relationship between GPP and SIF is primarily driven by the common APAR term. $\Theta_{\rm f}$ is expected to co-vary with LUE_p under high light conditions because of plant's protective mechanisms (Damm et al., 2010; Damm et al., 2015). The variations in $\Theta_{\rm f}$ are reflected in SIF but not necessarily in vegetation indices. The superiority of SIF over vegetation indices in monitoring drought stress and vegetation phenology has been demonstrated in previous studies (Damm et al., 2010; Damm et al., 2015; Daumard et al., 2010; Joiner et al., 2014; Rascher et al., 2015; Sun et al., 2015; Wang et al., 2016; Yoshida et al., 2015).

Several studies have investigated the relationships between GPP and satellite-derived SIF for different biomes (Frankenberg et al., 2011; Guanter et al., 2012; Joiner et al., 2014; Parazoo et al., 2014). The satellite-derived SIF data were mainly derived from the Greenhouse Gases Observing Satellite (GOSAT) and the Global Ozone Monitoring Experiment 2 (GOME-2). Frankenberg et al. (2011) showed strong linear relationships between GOSAT SIF and gridded GPP products, suggesting that SIF could better predict GPP than some approaches based on traditional vegetation indices, ancillary data, and model assumptions. Guanter et al. (2012) found that there was strong

correlation between GOSAT SIF and gridded GPP products, and the slope of the relationship varied with biome. Another study indicated that GOME-2 SIF could better track vegetation phenology for several different biomes than existing models and satellite data products (Joiner et al., 2014). Although these findings are promising, the GPP data used to evaluate the SIF data were mainly from gridded data products (e.g., upscaled GPP products, the MODIS GPP product) estimated by data-driven (Jung et al., 2011) or LUE (Zhao et al., 2005) approaches. Most ecosystems are highly heterogeneous at spatial scales larger than 5-10 km (Duveiller and Cescatti, 2016). The evaluation of GOSAT and GOME-2 SIF using ecosystem-level GPP derived from eddy covariance (EC) flux towers are hindered by the coarse spatial resolution of these SIF products $(40 \times 80 \text{ km}^2 \text{ for GOME-2})$ and 10 km diameter for GOSAT) and the resulting large scale mismatch between satellite and tower footprints. The recent release of the finer-resolution SIF products from NASA's Orbiting Carbon Observatory-2 (OCO-2) (Frankenberg et al., 2014) makes it possible to directly link satellitederived SIF with tower GPP at the ecosystem scale for the first time.

The OCO-2 was launched on July 2, 2014 and was the replacement for the Orbiting Carbon Observatory (OCO) lost in launch failure in 2009. OCO-2 incorporates three high resolution spectrometers that simultaneously measure reflected sunlight in the near infrared CO2 absorption bands near 1.61 and 2.06 μm, and in molecular oxygen (O2) A-Band at 0.76 µm (Frankenberg et al., 2014). The sun-synchronous orbit with 1:30 p.m. local overpass time enables the retrieval of far-red SIF at mid-day time similar to the GOSAT but with higher fidelity and much reduced standard error. The biggest advancement of OCO-2 over GOME-2 and GOSAT lies in the dramatic increase in measurement frequency and much smaller ground-pixel sizes (1.3 × 2.25 km²) (Frankenberg et al., 2014). OCO-2 measurements are collected in Nadir and Glint viewing mode alternatively and a special Target observation mode with a repeat frequency of approximately 16 days (Frankenberg et al., 2014). The footprint of OCO-2 is close to that of EC flux towers. and therefore OCO-2 provides unique opportunities for better investigating the relationships between SIF and GPP (Frankenberg et al., 2016). Two recent studies performed the first assessments of the OCO-2 SIF and tower GPP relationships for corn (Wood et al., 2017) and grassland ecosystems (Verma et al., 2017). Wood et al. (2017) found consistently strong linear GPP-SIF relationships at different timescales for corn ecosystems. Verma et al. (2017) examined how environmental conditions affected the GPP-SIF relationship for a grassland ecosystem at OCO-2 overpass time. The relationship between OCO-2 SIF and tower GPP has not been examined for forest ecosystems.

In this study, we examined the relationships between SIF from OCO-2 and flux tower GPP in temperate forests. We chose two study sites (Park Falls and Willow Creek, Wisconsin, U.S.A.) based on the availability of intensive OCO-2 observations and EC flux tower measurements from 2014 to 2016. The Park Falls is one of the primary sites for the OCO-2 calibration/validation. The OCO-2 collects data over these calibration/validation sites in the Target mode and provides a large number of soundings in the vicinity of the targeted landscape, which reduces the impact of random errors and provides a valuable opportunity for conducting a more robust evaluation of the relationships between OCO-2 SIF and tower GPP. To our knowledge, this study provides the first evaluation of the OCO-2 SIF collected in the Target mode and the first assessment of the OCO-2 SIF and tower GPP relationship for forest ecosystems. First, we examined the relationships between tower GPP and OCO-2 SIF at two retrieval bands (757 and 771 nm) and two timescales (OCO-2 overpass time and daily timescale). Second, we evaluated the relationships between tower GPP and MODIS vegetation indices (NDVI and EVI) to assess how OCO-2 SIF performs compared to these widely-used vegetation indices. Third, we further investigated the correlations of OCO-2 SIF with MODIS fPAR, APAR, and APAR $\times fT_{\min} \times fVPD$, i.e. the product of APAR and two environmental scaling factors for low temperature stress and water stress. Fourth, we evaluated the performance of a hyperbolic model based on

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