Remote Sensing of Environment 209 (2018) 808–823

Contents lists available at ScienceDirect

Remote Sensing of Environment

journal homepage: www.elsevier.com/locate/rse

Overview of Solar-Induced chlorophyll Fluorescence (SIF) from the Orbiting Carbon Observatory-2: Retrieval, cross-mission comparison, and global monitoring for GPP

Ying Sun[a,b,*], Christian Frankenberg[c,a,**], Martin Jung[d], Joanna Joiner[e], Luis Guanter[f], Philipp Köhler[c], Troy Magney[a]

[a] Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA, United States
[b] School of Integrative Plant Science, Soil and Crop Sciences Section, Cornell University, Ithaca, NY, United States
[c] Division of Geological and Planetary Sciences, California Institute of Technology, Pasadena, CA, United States
[d] Max Planck Institute for Biogeochemistry, Jena, Germany
[e] NASA Goddard Space Flight Center, Greenbelt, MD, United States
[f] Helmholtz Centre Potsdam, German Research Centre for Geosciences, Potsdam, Germany

ARTICLE INFO

Keywords:
OCO-2
SIF
Photosynthesis
GPP
Carbon cycle

ABSTRACT

The Orbiting Carbon Observatory-2 (OCO-2), launched in July 2014, is capable of measuring Solar-Induced chlorophyll Fluorescence (SIF), a functional proxy for terrestrial gross primary productivity (GPP). Although its primary mission is to measure the column-averaged mixing ratio of CO_2 (X_{CO_2}) to constrain global carbon source/sink distribution, one of the OCO-2 spectrometers allows for a robust SIF retrieval solely based on solar Fraunhofer lines. Here we present a technical overview of the OCO-2 SIF product, aiming to provide the scientific community guidance on best practices for data analysis, interpretation, and application. This overview consists of the retrieval algorithms, OCO-2 specific bias correction, retrieval uncertainty evaluation, cross-mission comparison with other existing SIF products, and a global-scale examination of the SIF-GPP relationship. With the initial three years of data (September 2014 onward), we compared OCO-2 SIF with retrievals from Greenhouse Gases Observing Satellite (GOSAT) and Global Ozone Monitoring Experiment-2 (GOME-2), and examined its relationship with FLUXCOM and MODIS GPP datasets. Our results show that OCO-2 SIF, along with GOSAT products, closely resemble the mean spatial and temporal patterns of FLUXCOM GPP from regions to the globe. Compared with GOME-2, however, OCO-2 depicts a more realistic spatial contrast between the tropics and extra-tropics. The linear relationship between OCO-2 SIF and existing modeled GPP products diverges somewhat across biomes at the global scale, consistent with previous GOSAT or GOME-2 based findings when modeled GPP products were used, but in contrast to a consistent cross-biome SIF-GPP relationship obtained at flux tower sites with OCO-2 products. This contrast suggests a critical need to reconcile differences in diverse SIF and GPP products and the relationships among them. Overall, the OCO-2 SIF products are robust and valuable for monitoring the global terrestrial carbon cycle and for constraining the carbon source/sink strengths of the Earth system. Finally, insights are offered for future satellite missions optimized for SIF retrievals.

1. Introduction

Satellite measurements of steady-state Solar-Induced chlorophyll Fluorescence (SIF) open up a new avenue for monitoring terrestrial gross primary productivity (GPP) from space (Frankenberg et al., 2011b; Guanter et al., 2012; Joiner et al., 2013, Jung et al., 2011; Köhler et al., 2015; Y. Sun et al., 2017). Detecting SIF is also critical to accurate retrievals of trace gases such as column-averaged dry-air mole fraction of CO_2 (i.e., X_{CO_2}) (Frankenberg et al., 2012, 2011a). Global retrievals of satellite SIF have been achieved at various wavelengths with multiple space-borne instruments (Frankenberg et al., 2011b; Guanter et al., 2012; Joiner et al., 2013, 2011; Köhler et al., 2015). Existing instruments include the Fourier Transform Spectrometer (FTS) onboard the Japanese Greenhouse Gases Observing Satellite (GOSAT), the Global Ozone Monitoring Experiment-2 (GOME-2) onboard the European MetOp-A and MetOp-B, the SCanning Imaging Absorption

* Correspondence to: Y. Sun, School of Integrative Plant Science, Soil and Crop Sciences Section, Cornell University, Ithaca, NY, United States.
** Correspondence to: C. Frankenberg, Division of Geological and Planetary Sciences, California Institute of Technology, Pasadena, CA, United States.
E-mail addresses: ys776@cornell.edu (Y. Sun), cfranken@caltech.edu (C. Frankenberg).

https://doi.org/10.1016/j.rse.2018.02.016
Received 3 February 2018; Accepted 12 February 2018
Available online 27 February 2018

spectroMeter for Atmospheric CHartographY (SCIAMACHY) onboard ENVISAT, the Orbiting Carbon Observatory-2 (OCO-2), and the TROPOspheric Monitoring Instrument (TROPOMI) onboard Sentinel-5 Precursor (S5p).

The general principle for retrieving SIF is based on the in-filling of solar Fraunhofer lines, i.e., measuring the fractional depth of the Fraunhofer lines, which decreases in the presence of SIF emission from the Earth surface. This approach was originally proposed by Plascyk and Gabriel (1975) and evaluated by the in-filling of luminescence in a single deep Fraunhofer line. The first global SIF retrieval was achieved with GOSAT-FTS, by evaluating the in-filling of Fraunhofer lines located around 755 nm and 771 nm where the contamination from atmospheric scattering and absorption is minimized (Joiner et al., 2011; Frankenberg et al., 2011b; Guanter et al., 2012). The high spectral resolution of GOSAT-FTS (~0.025 nm) allows for resolving the narrow and isolated solar Fraunhofer lines, ensuring a robust and accurate retrieval. However, GOSAT has poor spatial and temporal data sampling. It acquires only one spectrum every 4 s and individual orbital tracks are hundreds of kilometers apart. This drawback hinders the continuous global mapping of SIF with GOSAT. Subsequent studies using GOME-2 and SCIAMACHY (Joiner et al., 2013, 2012; Köhler et al., 2015; Wolanin et al., 2015) showed that it is also possible to retrieve SIF with moderate spectral resolutions (~0.5 nm) by spectral fitting with a broad spectral window. Using a statistical approach based on principal component analysis (PCA) or singular value decomposition (SVD), SIF was inferred at 740 nm by fitting the window of 734–758 nm (Joiner et al., 2013) or 720–758 nm (Köhler et al., 2015). The PCA technique simplified the atmospheric radiative transfer modeling and enabled disentangling the spectral signatures of atmospheric absorption, surface reflectance, and fluorescence emission (Joiner et al., 2013). Although a broad spectral window fitting poses a challenge for completely eliminating the atmospheric impact on SIF, continuous spatial mapping became possible across the globe (Joiner et al., 2013; Köhler et al., 2015). In addition to the abovementioned efforts that focus on the far-red SIF retrieval, Joiner et al. (2016) developed a novel approach to estimate the SIF emission at the red spectral region. This approach utilizes the O_2 γ-band, which is relatively SIF free, to constrain the atmospheric impact on the absorption within the O_2 B band, thus isolating SIF in the O_2 B band from effects of scattering. This strategy improves the retrieval precision of red SIF as compared with fitting only Fraunhofer lines in the vicinity of the O_2 B band.

The availability of these SIF datasets has spurred a considerable number of applications of SIF to understand terrestrial ecosystem dynamics. Accurate interpretation and process attribution with SIF depend on specific data characteristics of each instrument (resolutions, retrieval precision, observational geometry, etc.). Such technical information has been provided for GOSAT (e.g., Frankenberg et al., 2011a, 2011b; Guanter et al., 2012), GOME-2 (e.g., Joiner et al., 2013; Köhler et al., 2015), and SCIAMACHY (e.g., Köhler et al., 2015). However, a comprehensive description of the OCO-2 SIF product is not yet provided to the community since OCO-2's launch in September 2014, although a growing number of OCO-2 SIF based studies have already been published recently (Köhler et al., 2017; Li et al., 2018; Y. Sun et al., 2017; Verma et al., 2017; Wood et al., 2017). This study aims to provide a technical overview of the OCO-2 SIF retrieval, in order to help users understand the data quality, advantage and limitations relative to other existing products. For this purpose, this paper will use the operational collection of OCO-2 measurements, different from Frankenberg et al. (2014), which used pre-launch synthetic simulations to assess the radiometric performance of the instrument. Y. Sun et al. (2017) has summarized the unique new research opportunities enabled by OCO-2 SIF, and this present paper focuses on the technical details of this dataset.

The paper is structured as follows: Section 2 provides a technical description of the OCO-2 SIF products, consisting of an OCO-2 mission overview, the retrieval algorithm, instrument "offset" correction, and quality control. Note the retrieval algorithm (Section 2.2) is not OCO-2 specific but is identical to the one implemented for GOSAT. It can also readily be applied to future missions that employ spectrometers of similar characteristics. It is included here for the sake of completeness to benefit readers. The correction of instrument artifacts (Section 2.5) is a critical step specific to the OCO-2 grating spectrometers and has to be carefully accounted for to ensure unbiased SIF retrieval. Section 3 describes the cross-comparison schemes among different missions that have the capability for SIF retrieval. Section 4 reports the results on the SIF cross-mission comparison and on the SIF-GPP relationships. The latter aspect has been intensively investigated for GOSAT and GOME-2, thus not inherently new to OCO-2; but it is included in this overview paper so that the SIF community can gain a complete picture about the OCO-2 SIF product and its capability/limitations in constraining GPP.

2. Description of the OCO-2 SIF product

2.1. The OCO-2 mission

OCO-2 flies in a sun-synchronous orbit with a local overpass time at 1:30 pm. The instrument consists of three grating spectrometers, recording high-resolution radiance spectra in three bands: the O_2-A band (757–775 nm, Full Width at Half Maximum FWHM = 0.042 nm), a weak CO_2 absorption band (1594–1627 nm, FWHM = 0.076 nm), and a strong CO_2 absorption band (2043–2087 nm, FWHM = 0.097 nm). The O_2-A band spectrometer is utilized for OCO-2 SIF retrieval as it 1) overlaps with the SIF emission spectrum (i.e., 660–850 nm) and 2) covers a few relatively deep solar Fraunhofer lines. Each spectrometer provides eight independent cross-track spectra, with each spectrum having a nominal spatial resolution of $1.3 \times 2.25\text{km}^2$ (denoted as footprint) at nadir. These footprints together cover a maximum ~10 km-wide full swath. Note that due to slit rotation, the effective swath narrows near the equator, where eight footprints repeat the same ground pixel as the slit is aligned exactly along track.

In the original configuration, the viewing geometry of OCO-2 alternates every 16 days (instrument repeat cycle) between nadir and glint modes. Since July 2nd, 2015, the satellite viewing modes alternate from orbit to orbit, not between repeat cycles. The nadir mode follows a similar ground track during each repeat cycle, allowing for a reliable detection of variations over time. Compared to the glint mode, the nadir mode typically provides a slightly higher spatial resolution, a better signal-to-noise ratio (SNR) over land, and more useful soundings in regions impacted by clouds or with significant topography. The glint mode, relative to nadir, has varying east-west offsets. Spectra acquired from the glint mode have significantly higher SNR over the dark ocean (especially at high latitudes) due to the "bright" specular reflectance of solar radiation. Over land, however, glint measurements may underestimate SIF compared to nadir, because a more shaded fraction of the canopy may be observed (Frankenberg et al., 2014). In addition to the nadir and glint modes, there is a target mode which is occasionally switched on when the satellite overpasses ground validation sites. In this mode, a large number of temporally continuous measurements at different viewing zenith angles (VZA) is made, enabling research into the bidirectional effect of SIF. The present paper focuses on nadir spectra, as they provide the most consistent measurements in time.

The OCO-2 spectrometers acquire 24 spectra per second, an almost 100-fold increase in data acquisition frequency over GOSAT (one spectrum every 4 s). The spatial resolution of OCO-2 nominal footprint is $1.3 \times 2.25\text{km}^2$, much finer than GOSAT, GOME-2, and SCIAMACHY (Table 1 and Y. Sun et al., 2017). On average, OCO-2 acquires > 10^5 clear-sky soundings on land per day, a considerable increase in data acquisition. These marked improvements of OCO-2 enable more in-depth SIF-related studies than previously possible, for example, improved validation with ground measurements and detection of small-scale eco-physiological changes (Y. Sun et al., 2017). The sampling strategy, however, comes at a cost of spatial contiguity, as OCO-2 does