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Evaluating the predictive power of sun-induced chlorophyll fluorescence to estimate net photosynthesis of vegetation canopies: A SCOPE modeling study

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ABSTRACT

Progress in imaging spectroscopy technology and data processing can enable derivation of the complete sun-induced chlorophyll fluorescence (SIF) emission spectrum. This opens up opportunities to fully exploit the use of the SIF spectrum as an indicator of photosynthetic activity. Simulations performed with the coupled fluorescence–photosynthesis model SCOPE were used to determine how strongly canopy-leaving SIF can be related to net photosynthesis of the canopy (NPC) for various canopy configurations. Regression analysis between SIF retrievals and NPC values produced the following general findings: (1) individual SIF bands that were most sensitive to NPC were located around the first emission peak (SIF_{red}) for heterogeneous canopy configurations (i.e., varying biochemistry, leaf, canopy variables); (2) using two SIF retrieval bands, e.g. O_2-B at 687 nm and O_2-A at 760 nm, or the red and NIR emission peaks at 685 nm and 740 nm, led to stronger correlations than using only one band; (3) using the O_2-B and the O_2-A SIF retrieval bands was at least as effective as using the two emission peaks; (4) superior correlations were achieved by using the four main SIF retrieval bands (Hα, O_2-B, water vapor, O_2-A); and (5) further improvements may be obtained by exploiting the full SIF profile and by using an adaptive, nonlinear regression algorithm such as Gaussian processes regression (GPR). Relationships can be due to variation in photosynthetic capacity (V_{cmo}), but also from variation in leaf optical and canopy structural variables such as chlorophyll content and leaf area index. Overall, modeling results suggest that sampling the SIF profile in at least both O_2-B and O_2-A bands enables quantification photosynthetic activity of vegetation with high accuracy.

1. Introduction

Sun-induced fluorescence (SIF) emitted by chlorophyll molecules is one of three main de-excitation mechanisms for energy captured by light harvesting pigments in plants. SIF emitted by vegetation is seen as a meaningful indicator of plant stress (Van Wittenberghe et al., 2013), instantaneous plant photosynthetic function (e.g., carbon fixation), and possibly gross primary productivity (GPP) at the ecosystem scale (Porcar-Castell et al., 2014).

Although the SIF flux emitted from the canopy is relatively small compared to reflected sunlight (about 1–5% in the near infrared; NIR), it is a broadband spectrum that typically spans about 650–800 nm (but which can also extend somewhat below or above that range, e.g., 640–850 nm), and which contains useful information on the photosynthetic process (Franck, Juneau, & Popovic, 2002; Lichtenthaler & Rinderle, 1988). Even though the canopy will produce different SIF spectra under different environmental and structural conditions, the shape of SIF spectra preserves typical features. In general, the SIF spectrum is composed of two peaks, one located in the red (SIF_{red}) spectral region with a maximum around 685 nm that is mainly attributed to the fluorescence emission of Photosystem II (PSII), and the other located in the NIR (SIF_{NIR}) with a maximum around 740 nm that is attributable to both Photosystem I (PSI) and PSII (Baker, 2008; Papageorgiou & Govindjee, 2004).

With the advent of imaging spectrometers, the retrieval of SIF using remote sensing technologies has become a novel area of research (Alonso et al., 2007; Guanter et al., 2010; Meroni et al., 2009, 2010) aimed primarily at mapping SIF from the site-specific (Damm et al., 2014; Daumard et al., 2012; Moya, Daumard, Moise, Ounis, & Goulas,

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2006; Perez-Priego, Zarco-Tejada, Miller, Sepulcre-Canto, & Fereres, 2005; Zarco-Tejada, Gonzalez-Dugo, & Berni, 2012; Zarco-Tejada, Morales, Testi, & Villalobos, 2013) to the global scale (Frankenberg et al., 2011; Joiner et al., 2011). In general, two strategies to extract SIF from passive detection methods have been pursued in recent years, exploiting either atmospheric (telluric) absorption features due to oxygen in the O_2-A absorption region at 760 nm (Alonso et al., 2007; Guanter et al., 2010; Meroni et al., 2010), or solar Fraunhofer lines, which are narrow dark lines (absorption features) in the solar spectrum in which irradiance is strongly reduced (e.g. in the NIR 740–770 nm spectral window) (Frankenberg et al., 2011; Guanter et al., 2012). Regardless of the retrieval strategy, current remote sensing approaches have mostly emphasized the second emission peak region (SIF_{NIR}) for photosynthetic quantification, especially from satellite-based atmospheric sensors. For example, Frankenberg et al. (2011) and Guanter et al. (2012) linked monthly-aggregated global SIF_{NIR} observations with global GPP products using (biome-specific) linear relationships. More recently, at the local scale, Damm, Guanter, Paul-Limoges, et al. (2015) linked airborne SIF_{NIR} measurements with eddy covariance flux tower GPP data and found that relationships were not linear but asymptotic when instantaneous rather than temporally aggregated measured data were used, and relationships were also ecosystem-specific.

One reason for the focus on the SIF_{NIR} has been the absence of spaceborne sensors spectrally optimized to capture the full SIF emission spectrum. To fill this gap, the European Space Agency (ESA) has been conducting Phase A/B1 evaluations of a candidate Earth Explorer mission dedicated to measurement of SIF in terrestrial vegetation. The Fluorescence Explorer (FLEX) satellite, equipped with a Fluorescence Imaging Spectrometer (FLORIS) onboard, has recently been approved as ESA's Earth Explorer 8 mission (ESA, 2015). FLEX will operate in a tandem mission with ESA's Sentinel-3 satellite, the latter to provide atmospheric and land surface data needed for atmospheric corrections and accurate SIF characterizations. FLORIS will measure the radiance between 500 and 780 nm with a bandwidth between 0.3 nm and 2 nm (depending on wavelength), providing images with a 150 km swath and 300 m pixel size (Kraft et al., 2013; Moreno, Asner, Bach, et al., 2006). Such finely resolved spectral sampling will allow retrieval of the full broadband fluorescence emission spectrum and related products such as F_{total} (i.e., integral of the fluorescence broadband spectrum). In addition, a novel airborne imaging spectrometer *HyPlant* has become available recently which demonstrates the potential of a FLORIS-type sensor (Rascher et al., 2015). *HyPlant* has an ultra-high spectral resolution in the red and near-infrared spectral region (0.26 nm FWHM (Full Width at Half Maximum) in the 670–780 nm spectral range). This allows quantification of sun-induced fluorescence fluxes in physical units for SIF_{red} and SIF_{NIR} (Rossini et al., 2015), and eventually over the full SIF spectral region at a local scale. Another airborne experiment demonstrated that GPP is most strongly related to SIF_{red} at the O_2-B absorption band (Cheng et al., 2013), possibly due to the relevance of the red band to photosystem II processes (Baker, 2008).

Additional advances in signal retrieval and data processing are evident. Developments include the use of multiple absorption lines in both emission peak regions for SIF retrievals, and simulations of the influences of different atmospheric conditions (Liu & Liu, 2014). For example, Zhao et al. (2014) examined SIF retrieval in five absorption lines to allow reconstruction of the full SIF emission between 650 and 850 nm based on simulated data. Also within the FLEX scientific studies, a spectral fitting method has been developed that, when combined with an atmospheric correction algorithm, is able to reconstruct the full SIF spectrum directly from top of atmosphere (TOA) radiance data (Cogliati et al., 2015). Reconstruction of the full SIF spectrum will allow calculation of some other meaningful parameters relevant to detection of plant stress status, such as the spectral positions and FWHM of the SIF_{red} and SIF_{NIR} peaks, and the area under the SIF emission curve (Subhash & Mohanan, 1997; Zhao et al., 2014).

The FLEX scientific studies have also investigated radiative transfer modeling of the SIF signal through the leaf and canopy based on explicit leaf physiological descriptions. The SCOPE (Soil-Canopy Observation, Photosynthesis and Energy Balance) model (Van der Tol, Berry, Campbell, & Rascher, 2014; Van der Tol, Verhoef, Timmermans, Verhoef, & Su, 2009) has been coupled with new leaf fluorescence modules (resulting in Version 1.53). SCOPE combines the functionality of a Soil–Vegetation–Atmosphere-Transfer (SVAT) model with radiative transfer of reflected and emitted (thermal and fluorescent) radiation and enables the theoretical quantification of the canopy-leaving SIF broadband spectrum and canopy fluxes, such as the net photosynthesis of the canopy (NPC).

Now that derivation of the full SIF spectrum is possible, it creates opportunities to utilize more effectively the spectral information content related to NPC. An imminent requirement is to identify which SIF wavelengths are most sensitive to NPC. This leads to the main objective of this work: to analyze the sensitivity of single wavelengths, as well as combinations of SIF retrieval bands in estimation of NPC for various canopy configurations.

For this purpose, a SCOPE modeling study was applied. Simulations of canopy-leaving SIF and NPC outputs were conducted for different combinations of biochemical, leaf, canopy and micrometeorological variables. Simulated SIF spectra were subsequently analyzed with respect to their predictive power in estimating NPC. Specifically, the following aspects were investigated; (1) linear regression analysis between individual SIF bands and NPC outputs; (2) linear regression analysis between combined SIF bands and NPC outputs; and (3) adaptive, nonlinear machine learning regression between combined SIF bands and NPC outputs.

2. Materials and methods

2.1. SCOPE

The coupled fluorescence–photosynthesis model SCOPE simulates photosynthesis, radiative transfer in the leaf and canopy, and surface energy balance (Van der Tol et al., 2009, 2014). SCOPE recently became a virtual laboratory for studies on surface energy balance (Timmermans, Su, Van der Tol, Verhoef, & Verhoef, 2013), remote sensing thermal infrared measurements (Duffour, Olioso, Demarty, Van der Tol, & Lagouarde, 2015), and SIF-photosynthesis studies (Damm, Guanter, Paul-Limoges, et al., 2015; Verrelst et al., 2015; Zhang, Guanter, et al., 2014).

For photosynthesis, SCOPE uses either the model of Von Caemmerer (2000, 2013) or Collatz, Ball, Grivet, and Berry (1991), Collatz, Ribas-Carbo, and Berry (1992). These physiological models originally were developed to interpret measurements of leaf gas exchange. The main boundary conditions for photosynthesis are energy supply (light) and carbon dioxide diffusion into the leaf. The models calculate photosynthesis under the condition that these two aspects, the energy supply and the carbon dioxide flux, are in equilibrium. Electron transport (i.e., transfer of the energy supply) is calculated classically from active fluorescence measurements (e.g. Genty, Wonders, & Baker, 1990; Maxwell & Johnson, 2000; Weis & Berry, 1987). However, active techniques typically are only feasible in a laboratory or small scale field study due to requirements for saturating light flashes, and for modulation of the measuring light beam when fluorescence is assessed in natural outdoor conditions (Maxwell & Johnson, 2000; Van der Tol et al., 2014). For this reason, the photosynthesis model in SCOPE is complemented with these alternative predictive models for fluorescence that serve to simulate the fluorescence leaf emission efficiency, ε, as a function of weather conditions and photosynthesis parameters, normalized by the leaf fluorescence emission efficiency in (near) dark or pre-dawn conditions. The model of Van der Tol et al. (2014), is a semi-empirical model based upon field and laboratory experiments of unstressed